Access DB# 77853

526

SEARCH REQUEST FORM

Scientific and Technical Inf rmation Center

Requester's Full Name: PATEL SUDHAKER Examiner #: 77018 Date: 10/12/02

Art Unit: 1624 Phone Number 30 84709 Serial Number: 10/085,368

Mail Box and Bldg/Room Location: CM1 4E17 Results Format Preferred (circle): PAPER DISK E-MAIL

4E12

If more than one search is submitted, please prioritize searches in order of need. mej

****

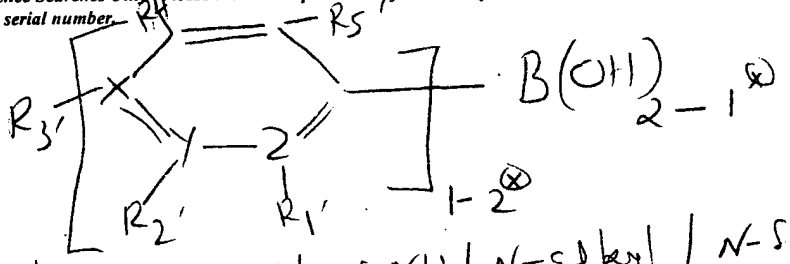
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: PROCESS FOR PREPARING BORONIC & BORONIC ACIDS

Inventors (please provide full names): ANDREAS HEUDT et al

Earliest Priority Filing Date: 3/2/2001

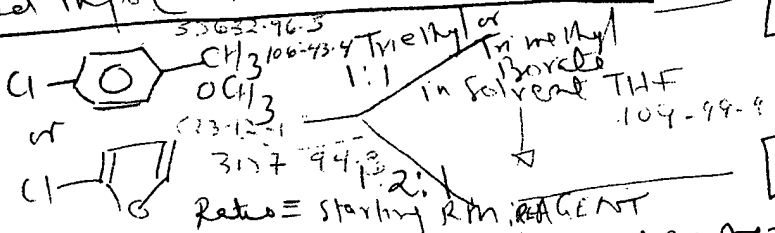
**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*



X/Y/Z = CH/ or NH/ N-alkyl / N-SiMe3 / S/O

i.e. X=Y-Z= form Phenyl / Pyridine / 1,4 or 1,3 or 1,2-Diazine or 1,2; 1,3; 1,4 - Oxazine or 1,2; 1,3; 1,4 - Thiazine

Need info on PROCESS OF MAKING



Ratio = Starting RM : REAGENT

need 4 hrs hitits abs total in CAPLUS/CAREACT

1624

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STAFF USE ONLY

Searcher: _____

Searcher Phone #: _____

Searcher Location: _____

Date Searcher Picked Up: 10/21

Date Completed: 10/24

Searcher Prep & Review Time: 17

Clerical Prep Time: _____

Online Time: 95

Point of Contact:
Alexandra Waclawiw
Technical Info. Specialist
CM1 6A02 Tel: 308-4491

Type of Search

NA Sequence (#) _____

AA Sequence (#) _____

Structure (#) 4

Bibliographic _____

Litigation _____

Fulltext _____

Patent Family _____

Other _____

Vendors and cost where applicable

STN $643.00

Dialog _____

Questel/Orbit _____

Dr.Link _____

Lexis/Nexis _____

Sequence Systems _____

WWW/Internet _____

Other (specify) _____

RECEIVED OCT 11 2002 (STIC)

PTO-1590 (8-01)

=> d his

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     (FILE 'REGISTRY' ENTERED AT 08:42:09 ON 24 OCT 2002)
                DEL HIS Y
                ACT PATEL10/A
               ---------
L1              STR
L2         63892 SEA FILE=REGISTRY SSS FUL L1
               ---------
                ACT PATEL4/A
               ---------
L3              STR
L4              STR
L5   (     63892)SEA FILE=REGISTRY SSS FUL L4
L6          3625 SEA FILE=REGISTRY SUB=L5 SSS FUL L3
               ---------
                ACT PATELREACT/A
               ---------
L7              STR
L8              STR
L9   (     63892)SEA FILE=REGISTRY SSS FUL L8
L10  (      3625)SEA FILE=REGISTRY SUB=L9 SSS FUL L7
L11  (     60267)SEA FILE=REGISTRY ABB=ON  PLU=ON  L9 NOT L10
L12             STR
L13         1195 SEA FILE=REGISTRY SUB=L11 SSS FUL L12
               ---------
L14            4 S 53632-96-5 OR 106-43-4 OR 3187-94-8 OR 623-12-1

     FILE 'HCAPLUS' ENTERED AT 09:16:51 ON 24 OCT 2002

     FILE 'REGISTRY' ENTERED AT 09:16:53 ON 24 OCT 2002
                E LITHIUM/CN
L15             1 S E3
                E THF/CN
L16             1 S E3

     FILE 'HCAPLUS' ENTERED AT 09:17:12 ON 24 OCT 2002
L17         4094 S L6/P OR L6 (L) (PREPN OR PREPAR? OR MANUF? OR MRF# OR MFG# OR
L18         5710 S L13 (L) (RCT OR RACT)/RL
L19          508 S L17 AND L18
L20         2692 S L14
L21           30 S L17 AND L20
L22       288334 S L15 OR LI OR LITHI? OR L16 OR THF
L23            4 S L19 AND L20
L24           58 S L19 AND L22
L25            3 S L24 AND SOLV?

     FILE 'REGISTRY' ENTERED AT 09:24:52 ON 24 OCT 2002
                E TRIETHYLAMINE/CN
L26             1 S E3
                E DIETHYL ETHER/CN
L27             1 S E3
                E DI-N-BUTYL ETHER/CN
L28             1 S E3
                E TERT-BUTYL METHYL ETHER/CN
L29             1 S E3
                E XYLENE/CN
L30             1 S E3
                E TOLUENE/CN
L31             1 S E3
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L32 6 S L26-L31

FILE 'HCAPLUS' ENTERED AT 09:26:16 ON 24 OCT 2002
L33 98857 S L32
L34 7 S L33 AND L19
L35 13 S L34 OR L25 OR L23
L36 26 S L21 NOT L35

```
=> fil reg
FILE 'REGISTRY' ENTERED AT 09:27:20 ON 24 OCT 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   22 OCT 2002  HIGHEST RN 464152-74-7
DICTIONARY FILE UPDATES:  22 OCT 2002  HIGHEST RN 464152-74-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d que stat l2
L1                  STR
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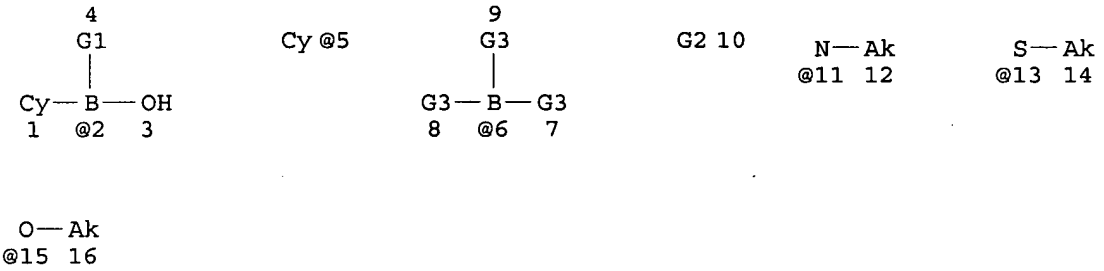


```
VAR G1=OH/5
VAR G2=6/2
VAR G3=11/13/15/X
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  12
CONNECT IS E1  RC AT  14
CONNECT IS E1  RC AT  16
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   1
GGCAT   IS MCY  UNS  AT   5
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  16

STEREO ATTRIBUTES: NONE
L2        63892 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 299270 ITERATIONS                 63892 ANSWERS
SEARCH TIME: 00.00.06
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broad search includes both I, II, and BWW

```
=> d questat 16
L3                  STR
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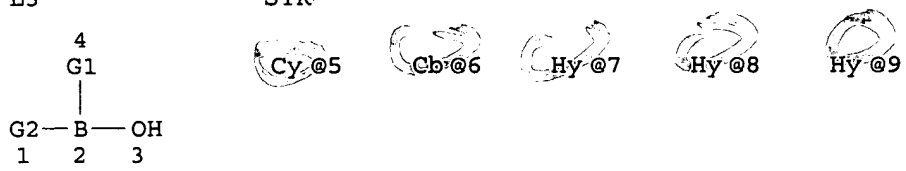


```
VAR G1=OH/5
VAR G2=6/7/8/9
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   5
GGCAT   IS MCY  UNS  AT   6
GGCAT   IS MCY  UNS  AT   7
GGCAT   IS MCY  UNS  AT   8
GGCAT   IS MCY  UNS  AT   9
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E5 C  E1 N  AT   7
ECOUNT  IS E4 C  E1 N  E1 O  AT   8
ECOUNT  IS E4 C  E1 N  E1 S  AT   9

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   9

STEREO ATTRIBUTES: NONE
L4                  STR
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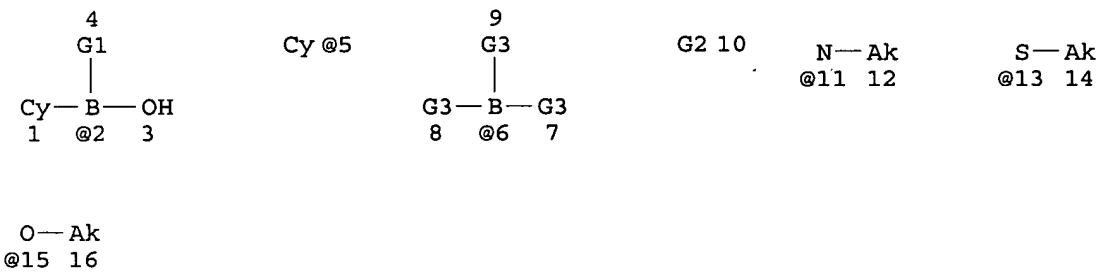



```
VAR G1=OH/5
VAR G2=6/2
VAR G3=11/13/15/X
NODE ATTRIBUTES:
CONNECT IS E1  RC AT  12
CONNECT IS E1  RC AT  14
CONNECT IS E1  RC AT  16
DEFAULT MLEVEL IS ATOM
GGCAT   IS MCY  UNS  AT   1
GGCAT   IS MCY  UNS  AT   5
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  16
```

STEREO ATTRIBUTES: NONE
L5 (63892)SEA FILE=REGISTRY SSS FUL L4
L6 3625 SEA FILE=REGISTRY SUB=L5 SSS FUL L3

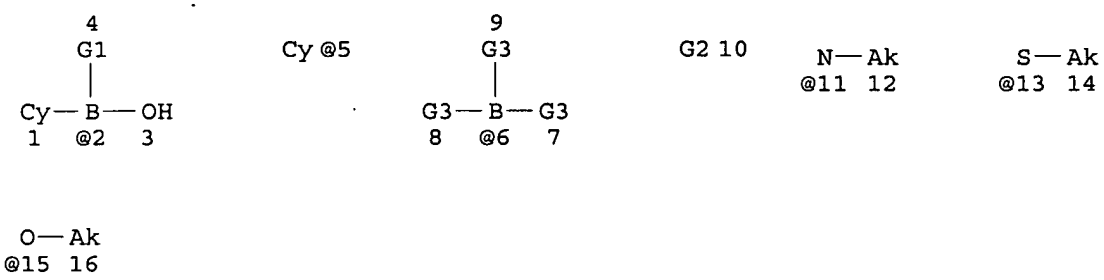
100.0% PROCESSED 6872 ITERATIONS 3625 ANSWERS
SEARCH TIME: 00.00.01

=> d que stat l13
L7 STR

VAR G1=OH/5
VAR G2=6/7/8/9
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY UNS AT 5
GGCAT IS MCY UNS AT 6
GGCAT IS MCY UNS AT 7
GGCAT IS MCY UNS AT 8
GGCAT IS MCY UNS AT 9
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E5 C E1 N AT 7
ECOUNT IS E4 C E1 N E1 O AT 8
ECOUNT IS E4 C E1 N E1 S AT 9

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE
L8 STR

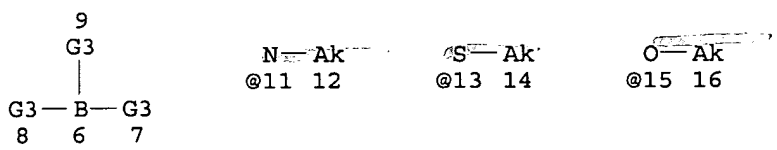


VAR G1=OH/5
VAR G2=6/2
VAR G3=11/13/15/X
NODE ATTRIBUTES:
CONNECT IS E1 RC AT 12
CONNECT IS E1 RC AT 14
CONNECT IS E1 RC AT 16
DEFAULT MLEVEL IS ATOM
GGCAT IS MCY UNS AT 1
GGCAT IS MCY UNS AT 5

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE
L9 (63892)SEA FILE=REGISTRY SSS FUL L8
L10 (3625)SEA FILE=REGISTRY SUB=L9 SSS FUL L7
L11 (60267)SEA FILE=REGISTRY ABB=ON PLU=ON L9 NOT L10
L12 STR



VAR G3=11/13/15/X
NODE ATTRIBUTES:
CONNECT IS E3 RC AT 6
CONNECT IS E1 RC AT 12
CONNECT IS E1 RC AT 14
CONNECT IS E1 RC AT 16
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE
L13 1195 SEA FILE=REGISTRY SUB=L11 SSS FUL L12

100.0% PROCESSED 60267 ITERATIONS 1195 ANSWERS
SEARCH TIME: 00.00.03

=> d que l14
L14 4 SEA FILE=REGISTRY ABB=ON PLU=ON 53632-96-5 OR 106-43-4 OR 3187-94-8 OR 623-12-1

=> d rn cn l14 1-4

L14 ANSWER 1 OF 4 REGISTRY COPYRIGHT 2002 ACS
RN **53632-96-5** REGISTRY
CN Benzene, 1-chloro-4-methyl-, radical ion(1+) (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-Chloro-4-methylbenzene ion(1+)
CN p-Chlorotoluene cation radical
CN p-Chlorotoluene radical cation
CN p-Chlorotoluene(1+)

L14 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2002 ACS
RN **3187-94-8** REGISTRY
CN Furan, 2-chloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-Chlorofuran

CN 2-Furanyl chloride

L14 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2002 ACS
RN **623-12-1** REGISTRY
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Anisole, p-chloro- (6CI, 7CI, 8CI)
OTHER NAMES:
CN 1-Chloro-4-methoxybenzene
CN 1-Methoxy-4-chlorobenzene
CN 4-Chloroanisole
CN 4-Chlorophenol methyl ether
CN 4-Methoxychlorobenzene
CN 4-Methoxyphenyl chloride
CN Anisyl chloride
CN p-Chloroanisole
CN p-Chloromethoxybenzene
CN p-Chlorophenyl methyl ether
CN p-Methoxychlorobenzene
CN p-Methoxyphenyl chloride

L14 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2002 ACS
RN **106-43-4** REGISTRY
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Toluene, p-chloro- (8CI)
OTHER NAMES:
CN 1-Chloro-4-methylbenzene
CN 1-Methyl-4-chlorobenzene
CN 4-Chloro-1-methylbenzene
CN 4-Chlorotoluene
CN 4-Methylchlorobenzene
CN 4-Methylphenyl chloride
CN 4-Tolyl chloride
CN p-Chloromethylbenzene
CN p-Chlorotoluene
CN p-Methylchlorobenzene
CN p-Tolyl chloride
CN para-Chlorotoluene

=> d que l15;d l15
L15 1 SEA FILE=REGISTRY ABB=ON PLU=ON LITHIUM/CN

L15 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 7439-93-2 REGISTRY
CN **Lithium (7CI, 8CI, 9CI)** (CA INDEX NAME)
OTHER NAMES:
CN Lithium atom
CN Lithium element
MF Li
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC,

PIRA, PROMT, RTECS*, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VETU, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

Li

63552 REFERENCES IN FILE CA (1962 TO DATE)
5208 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
63615 REFERENCES IN FILE CAPLUS (1962 TO DATE)
5 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d que l16;d l16
L16 1 SEA FILE=REGISTRY ABB=ON PLU=ON THF/CN

L16 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 109-99-9 REGISTRY
CN Furan, tetrahydro- (7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 110: PN: WO02068584 PAGE: 57 claimed sequence
CN Butane .alpha.,.delta.-oxide
CN Butane, 1,4-epoxy-
CN Cyclotetramethylene oxide
CN Furanidine
CN Oxacyclopentane
CN Oxolane
CN Tetrahydrofuran
CN Tetramethylene oxide
CN **THF**
FS 3D CONCORD
DR 77392-70-2
MF C4 H8 O
CI COM
LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VETU, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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          17595 REFERENCES IN FILE CA (1962 TO DATE)
            500 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
          17631 REFERENCES IN FILE CAPLUS (1962 TO DATE)
              1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
```

Solvents

```
=> d que l32
L26             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  TRIETHYLAMINE/CN
L27             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  "DIETHYL ETHER"/CN
L28             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  "DI-N-BUTYL ETHER"/CN
L29             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  "TERT-BUTYL METHYL ETHER"/CN

L30             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  XYLENE/CN
L31             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  TOLUENE/CN
L32             6 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L26 OR L27 OR L28 OR L29 OR
                  L30 OR L31)


=> d l32 1-6

L32  ANSWER 1 OF 6  REGISTRY  COPYRIGHT 2002 ACS
RN   1634-04-4  REGISTRY
CN   Propane, 2-methoxy-2-methyl- (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Ether, tert-butyl methyl (6CI, 7CI, 8CI)
OTHER NAMES:
CN   1,1-Dimethylethyl methyl ether
CN   2-Methoxy-2-methylpropane
CN   2-Methyl-2-methoxypropane
CN   Methyl 1,1-dimethylethyl ether
CN   Methyl tert butyl ether
CN   Methyl tert-butyl ether
CN   Methyl tertiary butyl ether
CN   MTBE
CN   t-Butyl methyl ether
CN   tert-Butoxymethane
CN   tert-Butyl methyl ether
FS   3D CONCORD
MF   C5 H12 O
CI   COM
LC   STN Files:   AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS,
       BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS,
       CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*,
       DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2,
       HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS,
       NIOSHTIC, PDLCOM*, PHAR, PIRA, PROMT, RTECS*, SPECINFO, SYNTHLINE,
       TOXCENTER, ULIDAT, USPAT2, USPATFULL, VTB
         (*File contains numerically searchable property data)
     Other Sources:   DSL**, EINECS**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)


t-Bu— O— Me


**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
```

5042 REFERENCES IN FILE CA (1962 TO DATE)
14 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
5061 REFERENCES IN FILE CAPLUS (1962 TO DATE)
34 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L32 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2002 ACS
RN 1330-20-7 REGISTRY
CN Benzene, dimethyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN **Xylene (8CI)**
OTHER NAMES:
CN Dilan
CN Dimethylbenzene
CN Xylol
DR 8026-09-3
MF C8 H10
CI IDS, COM
LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VETU, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

2 (D1—Me)

14550 REFERENCES IN FILE CA (1962 TO DATE)
407 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
14582 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L32 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2002 ACS
RN 142-96-1 REGISTRY
CN Butane, 1,1'-oxybis- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Butyl ether (8CI)
OTHER NAMES:
CN 1,1'-Oxybisbutane
CN Butyl oxide
CN **Di-n-butyl ether**
CN Dibutyl ether
CN Dibutyl oxide
CN n-Butyl ether
FS 3D CONCORD
MF C8 H18 O
CI COM
LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, DIPPR*,

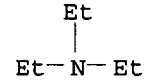
EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, SPECINFO, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

n-Bu—O—Bu-n

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2943 REFERENCES IN FILE CA (1962 TO DATE)
76 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
2947 REFERENCES IN FILE CAPLUS (1962 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L32 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2002 ACS
RN 121-44-8 REGISTRY
CN Ethanamine, N,N-diethyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN **Triethylamine (7CI, 8CI)**
OTHER NAMES:
CN (Diethylamino)ethane
CN N,N-Diethylethanamine
CN TEA
FS 3D CONCORD
DR 449752-61-8, 168277-99-4, 172227-74-6, 144514-14-7
MF C6 H15 N
CI COM
LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

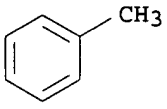


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

17060 REFERENCES IN FILE CA (1962 TO DATE)
702 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
17093 REFERENCES IN FILE CAPLUS (1962 TO DATE)
3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L32 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2002 ACS

RN 108-88-3 REGISTRY
CN Benzene, methyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN **Toluene (8CI)**
OTHER NAMES:
CN 1-Methylbenzene
CN Antisal 1a
CN CP 25
CN CP 25 (solvent)
CN Methacide
CN Methylbenzene
CN Methylbenzol
CN Phenylmethane
CN Toluol
FS 3D CONCORD
MF C7 H8
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIOGENES, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VETU, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

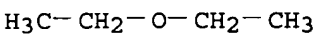


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

62040 REFERENCES IN FILE CA (1962 TO DATE)
660 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
62166 REFERENCES IN FILE CAPLUS (1962 TO DATE)
24 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L32 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2002 ACS
RN 60-29-7 REGISTRY
CN Ethane, 1,1'-oxybis- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Ether (6CI)
CN Ethyl ether (8CI)
OTHER NAMES:
CN 1,1'-Oxybisethane
CN 3-Oxapentane
CN Anaesthetic ether
CN Anesthesia ether
CN Anesthetic ether
CN **Diethyl ether**
CN Diethyl oxide

CN Ethoxyethane
CN Pronarcol
FS 3D CONCORD
DR 7578-39-4, 74446-43-8
MF C4 H10 O
CI COM
LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIPPR*, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, SPECINFO, TOXCENTER, TULSA, ULIDAT, USAN, USPAT2, USPATFULL, VETU, VTB
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

12264 REFERENCES IN FILE CA (1962 TO DATE)
125 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
12293 REFERENCES IN FILE CAPLUS (1962 TO DATE)
6 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 09:31:34 ON 24 OCT 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 24 Oct 2002 VOL 137 ISS 17
FILE LAST UPDATED: 23 Oct 2002 (20021023/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

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L4                STR
L5   (     63892)SEA FILE=REGISTRY SSS FUL L4
L6          3625 SEA FILE=REGISTRY SUB=L5 SSS FUL L3
L7                STR
L8                STR
L9   (     63892)SEA FILE=REGISTRY SSS FUL L8
L10  (      3625)SEA FILE=REGISTRY SUB=L9 SSS FUL L7
L11  (     60267)SEA FILE=REGISTRY ABB=ON  PLU=ON  L9 NOT L10
L12               STR
L13         1195 SEA FILE=REGISTRY SUB=L11 SSS FUL L12
L14            4 SEA FILE=REGISTRY ABB=ON  PLU=ON  53632-96-5 OR 106-43-4 OR
                  3187-94-8 OR 623-12-1
L15            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  LITHIUM/CN
L16            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  THF/CN
L17         4094 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L6/P OR L6 (L) (PREPN/OBI OR
                  PREPAR?/OBI OR MANUF?/OBI OR MRF#/OBI OR MFG#/OBI OR PREP/RL)
L18         5710 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L13 (L) (RCT OR RACT)/RL
L19          508 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17 AND L18
L20         2692 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L14
L22       288334 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L15 OR LI/OBI OR LITHI?/OBI
                  OR L16 OR THF/OBI
L23            4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L19 AND L20
L24           58 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L19 AND L22
L25            3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L24 AND SOLV?/OBI
L26            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  TRIETHYLAMINE/CN
L27            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  "DIETHYL ETHER"/CN
L28            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  "DI-N-BUTYL ETHER"/CN
L29            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  "TERT-BUTYL METHYL ETHER"/CN

L30            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  XYLENE/CN
L31            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  TOLUENE/CN
L32            6 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L26 OR L27 OR L28 OR L29 OR
                  L30 OR L31)
L33        98857 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L32
L34            7 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L33 AND L19
L35           13 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L34 OR L25 OR L23


=> d que nos l21;d his l36
L3                STR
L4                STR
L5   (     63892)SEA FILE=REGISTRY SSS FUL L4
L6          3625 SEA FILE=REGISTRY SUB=L5 SSS FUL L3
L14            4 SEA FILE=REGISTRY ABB=ON  PLU=ON  53632-96-5 OR 106-43-4 OR
                  3187-94-8 OR 623-12-1
L17         4094 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L6/P OR L6 (L) (PREPN/OBI OR
                  PREPAR?/OBI OR MANUF?/OBI OR MRF#/OBI OR MFG#/OBI OR PREP/RL)
L20         2692 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L14
L21           30 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17 AND L20

L36           26 S L21 NOT L35


=> d .ca hitstr l35 1-13;d .ca hitstr l36 1-26

L35  ANSWER 1 OF 13  HCAPLUS  COPYRIGHT 2002 ACS
ACCESSION NUMBER:         2002:671913  HCAPLUS
```

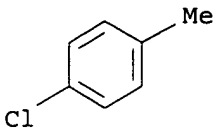
DOCUMENT NUMBER: 137:201430
TITLE: Process for preparing aromatic boronic and borinic acids
INVENTOR(S): Meudt, Andreas; Erbes, Michael; Forstinger, Klaus
PATENT ASSIGNEE(S): Clariant G.m.b.H., Germany
SOURCE: Eur. Pat. Appl., 9 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1236730	A2	20020904	EP 2002-3691	20020219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
DE 10110051	A1	20020912	DE 2001-10110051	20010302
JP 2002308883	A2	20021023	JP 2002-57278	20020304

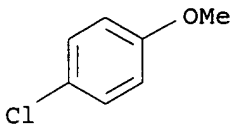
PRIORITY APPLN. INFO.: DE 2001-10110051 A 20010302

AB The process for prepn. of title compds., I and II (R1-R5 = H, Me, straight or branched C1-8 alkyl, F, CnH2n+1-f, n = 1-8, f = 1-2n+1 F, CH(OC1-5 alkyl)2, C(C1-5 alkyl), (OC1-5 alkyl), CH2(OC1-5 alkyl), CHMe(OC1-5 alkyl), C1-5 alkoxy, N(C1-5 alkyl)2, (un)substituted Ph, X, Y, Z = (un)substituted O, N, etc.), by the reaction of chloroarom. with BW'W''W''' (W', W'', W''' = C1-6 alkoxy, F, Cl, Br, I, diorganoamino, organothio, etc.), in a solvent at temp. of -100.degree. to 80.degree. is described. Thus, reaction of PhCl with Li in THF followed by treatment with B(OEt)3 and acidic hydrolysis gave 97% phenylboronic acid.

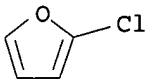
IC ICM C07F005-02
CC 29-4 (Organometallic and Organometalloidal Compounds)
IT 98-56-6, p-(Trifluoromethyl)chlorobenzene **106-43-4**, p-Chlorotoluene 108-90-7, Chlorobenzene, reactions **623-12-1**, p-Chloroanisole 625-98-9, m-Fluorochlorobenzene **3187-94-8**, 2-Chlorofuran
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and sequential reaction with boronate ester)
IT **98-80-6P**, Phenylboronic acid **768-35-4P**, m-Fluorophenylboronic acid **5720-05-8P**, p-Toluneboronic acid **5720-07-0P**, p-Anisylboronic acid 13331-23-2P, 2-Furylboronic acid **66117-64-4P**, Di(p-tolyl)borinic acid **128796-39-4P**, 4-(Trifluoromethyl)phenylboronic acid
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(**prepn.** of)
IT **121-43-7**, Trimethyl borate **150-46-9**, Triethyl borate
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(reaction with lithiated chloroaroms.)
IT **106-43-4**, p-Chlorotoluene **623-12-1**, p-Chloroanisole **3187-94-8**, 2-Chlorofuran
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and sequential reaction with boronate ester)
RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



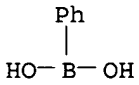
RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



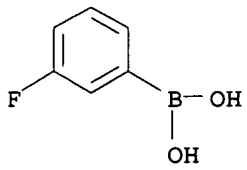
RN 3187-94-8 HCAPLUS
CN Furan, 2-chloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



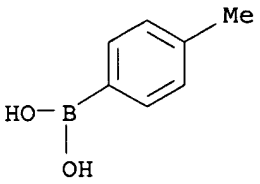
IT **98-80-6P**, Phenylboronic acid **768-35-4P**, m-Fluorophenylboronic acid **5720-05-8P**, p-Tolueneboronic acid **5720-07-0P**, p-Anisylboronic acid **66117-64-4P**, Di(p-tolyl)borinic acid **128796-39-4P**, 4-(Trifluoromethyl)phenylboronic acid
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



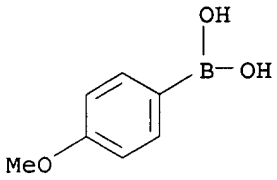
RN 768-35-4 HCAPLUS
CN Boronic acid, (3-fluorophenyl)- (9CI) (CA INDEX NAME)



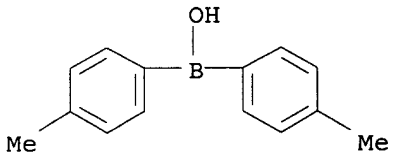
RN 5720-05-8 HCAPLUS
CN Boronic acid, (4-methylphenyl)- (9CI) (CA INDEX NAME)



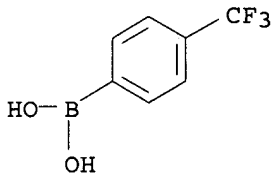
RN 5720-07-0 HCAPLUS
CN Boronic acid, (4-methoxyphenyl)- (9CI) (CA INDEX NAME)



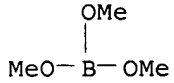
RN 66117-64-4 HCAPLUS
CN Borinic acid, bis(4-methylphenyl)- (9CI) (CA INDEX NAME)



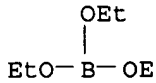
RN 128796-39-4 HCAPLUS
CN Boronic acid, [4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



IT **121-43-7**, Trimethyl borate **150-46-9**, Triethyl borate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction with lithiated chloroaroms.)
RN 121-43-7 HCAPLUS
CN Boric acid (H3BO3), trimethyl ester (8CI, 9CI) (CA INDEX NAME)



RN 150-46-9 HCAPLUS
CN Boric acid (H3BO3), triethyl ester (8CI, 9CI) (CA INDEX NAME)



L35 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:245404 HCAPLUS
DOCUMENT NUMBER: 137:185555
TITLE: Novel synthesis of arylboronic acids by electroreduction of aromatic halides in the presence of trialkyl borates
AUTHOR(S): Laza, Carine; Dunach, Elisabet; Serein-Spirau, Francoise; Moreau, Joel J. E.; Vellutini, Luc
CORPORATE SOURCE: Laboratoire Aromes, Syntheses et Interactions, Universite de Nice-Sophia Antipolis, Nice, 06108, Fr.
SOURCE: New Journal of Chemistry (2002), 26(4), 373-375
CODEN: NJCHE5; ISSN: 1144-0546
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A novel prepn. of aryl and heteroarylboronic acids by an electrochem. coupling reaction is described. It is based on the reductive coupling between arom. or heteroarom. halides and a trialkyl borate. The reactions are carried out in DMF or THF using sacrificial Al or Mg anodes in a single-compartment cell. Arylboronic acids were obtained with moderate to good selectivities and isolated yields.

CC 29-4 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 72

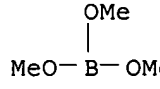
IT **121-43-7**, Trimethylborate **5419-55-6**, Triisopropylborate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(electroreductive coupling with arom. or heteroarom. halides to give arylboronic acids)

IT 96-43-5, 2-Chlorothiophene 106-38-7, p-Bromotoluene **106-43-4**, p-Chlorotoluene 108-86-1, Bromobenzene, reactions 576-83-0 578-57-4, o-Bromoanisole 1003-09-4, 2-Bromothiophene 3141-27-3, 2,5-Dibromothiophene 15499-27-1, 1-Butyl-4-Chloro-benzene 18246-28-1, 2-Bromo-5-trimethylsilylthiophene
RL: RCT (Reactant); RACT (Reactant or reagent)
(electroreductive coupling with trialkyl borate to give arylboronic acid)

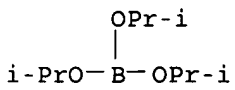
IT **98-80-6P 5720-05-8P 5720-06-9P**
5980-97-2P 6165-68-0P 138983-68-3P **145240-28-4P**
162607-17-2P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(**prepn.** of)

IT **121-43-7**, Trimethylborate **5419-55-6**, Triisopropylborate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(electroreductive coupling with arom. or heteroarom. halides to give arylboronic acids)

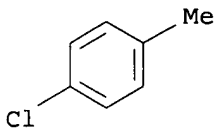
RN 121-43-7 HCAPLUS
CN Boric acid (H3BO3), trimethyl ester (8CI, 9CI) (CA INDEX NAME)



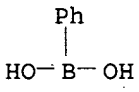
RN 5419-55-6 HCAPLUS
CN Boric acid (H3BO3), tris(1-methylethyl) ester (9CI) (CA INDEX NAME)



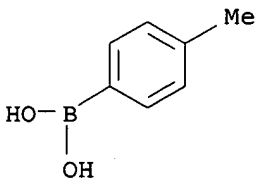
IT **106-43-4**, p-Chlorotoluene
RL: RCT (Reactant); RACT (Reactant or reagent)
(electroreductive coupling with trialkyl borate to give arylboronic acid)
RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



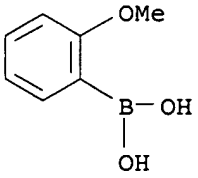
IT **98-80-6P 5720-05-8P 5720-06-9P**
5980-97-2P 145240-28-4P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(**prepn.** of)
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



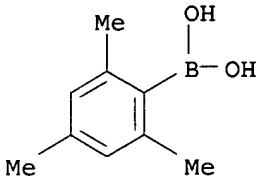
RN 5720-05-8 HCAPLUS
CN Boronic acid, (4-methylphenyl)- (9CI) (CA INDEX NAME)



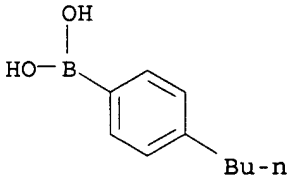
RN 5720-06-9 HCAPLUS
CN Boronic acid, (2-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 5980-97-2 HCAPLUS
CN Boronic acid, (2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



RN 145240-28-4 HCAPLUS
CN Boronic acid, (4-butylphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:113174 HCAPLUS
DOCUMENT NUMBER: 136:134913
TITLE: Preparation of phenylboronic acids and triphenylboroxins by Grignard reaction in nonether solvents
INVENTOR(S): Nakamura, Toshiki; Uchiyama, Nobuyuki; Kumamoto, Nobumitsu
PATENT ASSIGNEE(S): Hokko Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002047292	A2	20020212	JP 2000-227107	20000727

OTHER SOURCE(S): CASREACT 136:134913; MARPAT 136:134913
AB Title compds., useful as materials for biphenyl compds., are prepd. by Grignard reaction of B(OR)3 (R = alkyl, Ph) with PhMgX (the ring may be

mono- or disubstituted with alkyl, alkenyl, alkoxy, halo) at -10 to 15.degree. in nonether-type arom. solvents, followed by optional dehydration. Thus, a soln. of PhMgBr in THF-MePh mixt. was dropwise added to a soln. of B(OMe)3 in MePh at 0-5.degree. over 2 h and the reaction mixt. was left for 1 h to give 84.6% PhB(OH)2.

IC ICM C07F005-05
ICS C07F005-04

CC 29-4 (Organometallic and Organometalloidal Compounds)

IT **98-80-6P**, Phenylboronic acid
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(**prepn**. of phenylboronic acids and triphenylboroxins by Grignard reaction in nonether solvents)

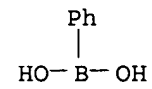
IT **1679-18-1P**, 4-Chlorophenylboronic acid **3262-89-3P**, Triphenylboroxin **5720-05-8P**, 4-Methylphenylboronic acid **5720-06-9P**, 2-Methoxyphenylboronic acid **5720-07-0P**, 4-Methoxyphenylboronic acid **10365-98-7P**, 3-Methoxyphenylboronic acid **16419-60-6P**, 2-Methylphenylboronic acid **17933-03-8P**, 3-Methylphenylboronic acid
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(**prepn**. of phenylboronic acids and triphenylboroxins by Grignard reaction in nonether solvents)

IT 95-46-5, 2-Bromotoluene 104-92-7, 4-Methoxybromobenzene 106-38-7, 4-Bromotoluene 106-39-8, 4-Chlorobromobenzene 108-86-1, Bromobenzene, reactions **121-43-7**, Trimethyl borate 578-57-4, 2-Methoxybromobenzene 591-17-3, 3-Bromotoluene 1095-03-0, Triphenyl borate 2398-37-0, 3-Methoxybromobenzene
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(prepn. of phenylboronic acids and triphenylboroxins by Grignard reaction in nonether solvents)

IT 71-43-2, Benzene, uses **108-88-3**, Toluene, uses
RL: NUU (Other use, unclassified); USES (Uses)
(solvent; prepn. of phenylboronic acids and triphenylboroxins by Grignard reaction in nonether solvents)

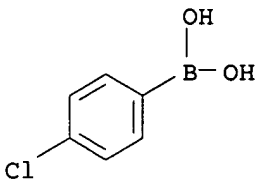
IT **98-80-6P**, Phenylboronic acid
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(**prepn**. of phenylboronic acids and triphenylboroxins by Grignard reaction in nonether solvents)

RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)

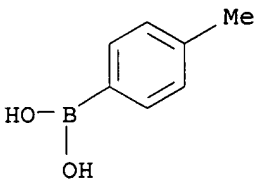


IT **1679-18-1P**, 4-Chlorophenylboronic acid **5720-05-8P**, 4-Methylphenylboronic acid **5720-06-9P**, 2-Methoxyphenylboronic acid **5720-07-0P**, 4-Methoxyphenylboronic acid **10365-98-7P**, 3-Methoxyphenylboronic acid **16419-60-6P**, 2-Methylphenylboronic acid **17933-03-8P**, 3-Methylphenylboronic acid
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(**prepn**. of phenylboronic acids and triphenylboroxins by Grignard reaction in nonether solvents)

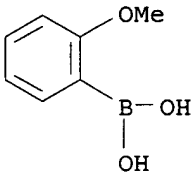
RN 1679-18-1 HCAPLUS
CN Boronic acid, (4-chlorophenyl)- (9CI) (CA INDEX NAME)



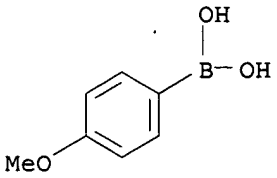
RN 5720-05-8 HCAPLUS
CN Boronic acid, (4-methylphenyl)- (9CI) (CA INDEX NAME)



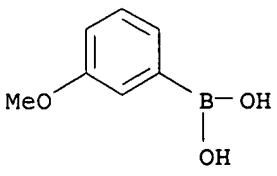
RN 5720-06-9 HCAPLUS
CN Boronic acid, (2-methoxyphenyl)- (9CI) (CA INDEX NAME)



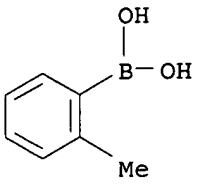
RN 5720-07-0 HCAPLUS
CN Boronic acid, (4-methoxyphenyl)- (9CI) (CA INDEX NAME)



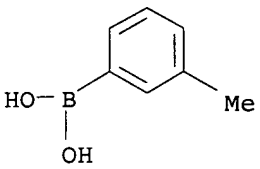
RN 10365-98-7 HCAPLUS
CN Boronic acid, (3-methoxyphenyl)- (9CI) (CA INDEX NAME)



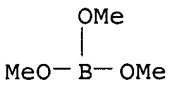
RN 16419-60-6 HCAPLUS
CN Boronic acid, (2-methylphenyl)- (9CI) (CA INDEX NAME)



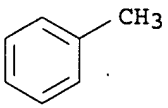
RN 17933-03-8 HCAPLUS
CN Boronic acid, (3-methylphenyl)- (9CI) (CA INDEX NAME)



IT **121-43-7**, Trimethyl borate
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(prepn. of phenylboronic acids and triphenylboroxins by Grignard reaction in nonether solvents)
RN 121-43-7 HCAPLUS
CN Boric acid (H3BO3), trimethyl ester (8CI, 9CI) (CA INDEX NAME)



IT **108-88-3**, Toluene, uses
RL: NUU (Other use, unclassified); USES (Uses)
(solvent; prepn. of phenylboronic acids and triphenylboroxins by Grignard reaction in nonether solvents)
RN 108-88-3 HCAPLUS
CN Benzene, methyl- (9CI) (CA INDEX NAME)



L35 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:905501 HCAPLUS
DOCUMENT NUMBER: 136:309948
TITLE: Synthesis and cross-coupling reactions of tetraalkylammonium organotrifluoroborate salts
AUTHOR(S): Batey, Robert A.; Quach, Tan D.
CORPORATE SOURCE: Department of Chemistry, University of Toronto,

Toronto, ON, M5S 3H6, Can.
SOURCE: Tetrahedron Letters (2001), 42(52), 9099-9103
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:309948

AB Treatment of organoboronic acids with HF generated an in situ tetracoordinate hydronium organotrifluoroborate species [PhBF3][H3O] which underwent counterion exchange with [Bu4N][OH]. The resultant tetraalkylammonium salts (I) are as air and moisture stable as their K organotrifluoroborate counterparts with the added advantage of being readily sol. in org. media. I underwent Pd-catalyzed Suzuki-Miyaura cross-couplings with a variety of aryl- and alkenyl halides under mild conditions. E.g., reaction of PhB(OH)2 with 3 equiv HF at room temp. for 1 h in H2O generated [PhBF3][H3O] which after counterion exchange with [Bu4N][OH] gave [PhBF3][Bu4N] (II) in 95% yield. II then underwent Pd-catalyzed Suzuki-Miyaura cross-coupling with PhI at room temp. (12 h) in presence of Pd(OAc)2/dppb catalyst and Cs2CO3 dissolved in DME/H2O (1:1) to give PhPh in quant. yield. Their Pd-catalyzed cross-coupling with acid halides was also possible for the generation of ketones. E.g., Pd-catalyzed cross-coupling of [Bu4N][C6H13CH:CHBF3] with p-AcC6H4Br under similar conditions to those above except at 50.degree. over 24 h gave p-(C6H13CH:CH)C6H4Ac in 87% yield.

CC 29-4 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 23, 25

IT 7732-18-5, Water, uses
RL: NUU (Other use, unclassified); USES (Uses)
(essential **solvent**; in prepn. of Pd-catalyzed cross-coupling reactions of organotrifluoroborate salts with alkenyl, aryl, and acid halides)

IT 92-52-4P, 1,1'-Biphenyl, preparation 92-91-1P 92-93-3P 103-36-6P 119-61-9DP, Diphenyl ketone, derivs. 613-37-6P 643-58-3P 769-57-3P 1008-88-4P 2051-62-9P 2113-58-8P 2920-38-9P, [1,1'-Biphenyl]-4-carbonitrile 3112-03-6P 3218-36-8P, p-Biphenylcarboxaldehyde 3976-35-0P 4423-09-0P 5002-13-1P 21308-81-6P 139502-80-0P 172035-84-6P 230647-85-5P 352206-56-5P 411206-71-8P, **Lithium** trifluoro(phenyl)borate 411206-72-9P, Sodium trifluoro(phenyl)borate 411206-74-1P, Tetrabutylphosphonium trifluoro(phenyl)borate 411206-85-4P 411206-92-3P 411206-93-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT 202409-79-8, **Lithium** tripropoxy(3-pyridinyl)borate
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of organotrifluoroborate salt from tripropoxyborate salt and hydrofluoric acid)

IT **1679-18-1**, (4-Chlorophenyl)boronic acid 12152-94-2, Ferrocenylboronic acid **13331-27-6**, (3-Nitrophenyl)boronic acid **149104-90-5**, (4-Acetylphenyl)boronic acid 214907-14-9, (1-Octenyl)boronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of organotrifluoroborate salts from boronic acids and hydrofluoric acid)

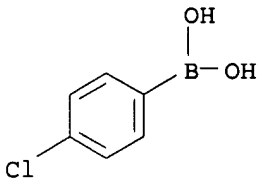
IT **5419-55-6**, Triisopropyl borate
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(reaction with bromopyridine)

IT **98-80-6**, Phenylboronic acid
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(reaction with hydrofluoric acid in **prepn**.

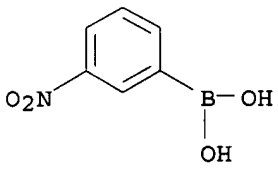
organotrifluoroborate salts and mechanism of cross-coupling reactions of organotrifluoroborate salts studied with)

IT **1679-18-1**, (4-Chlorophenyl)boronic acid **13331-27-6**, (3-Nitrophenyl)boronic acid **149104-90-5**, (4-Acetylphenyl)boronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of organotrifluoroborate salts from boronic acids and hydrofluoric acid)

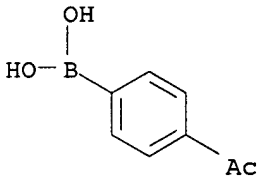
RN 1679-18-1 HCAPLUS
CN Boronic acid, (4-chlorophenyl)- (9CI) (CA INDEX NAME)



RN 13331-27-6 HCAPLUS
CN Boronic acid, (3-nitrophenyl)- (9CI) (CA INDEX NAME)

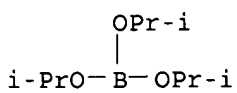


RN 149104-90-5 HCAPLUS
CN Boronic acid, (4-acetylphenyl)- (9CI) (CA INDEX NAME)



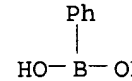
IT **5419-55-6**, Triisopropyl borate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction with bromopyridine)

RN 5419-55-6 HCAPLUS
CN Boric acid (H3BO3), tris(1-methylethyl) ester (9CI) (CA INDEX NAME)



IT **98-80-6**, Phenylboronic acid
RL: CPS (Chemical process); PEP (Physical, engineering or chemical

process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(reaction with hydrofluoric acid in **prepn.**
organotrifluoroborate salts and mechanism of cross-coupling reactions
of organotrifluoroborate salts studied with)
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:174453 HCAPLUS
DOCUMENT NUMBER: 134:193202
TITLE: Preparation of 1-Trifluoromethyl-2-alkylvinylaniline derivatives
INVENTOR(S): Jiang, Biao; Zhou, Jian; Zhang, Fangjiang; Ju, Wenjing
PATENT ASSIGNEE(S): Shanghai Inst. of Organic Chemistry, Chinese Academy of Sciences, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 12 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

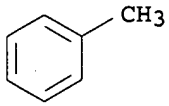
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1263084	A	20000816	CN 1999-127005	19991229

OTHER SOURCE(S): CASREACT 134:193202; MARPAT 134:193202
AB Title compds. [I; R = H, C1-5 alkyl; R1 = H, F, Cl, Br] are prepd. by acylating R1-aniline, brominating, substituting with tri-Bu borate, coupling with RCHXCHXCF3 or RCH:CXCF3 in org. solvent in the presence of inorg. base and transition complex catalyst at 25-80.degree. for 0.5-24 h, and hydrolyzing with acid. The transition complex catalyst is PdCl2(PPh3)2, Pd(PPh3)4, or NiCl3(PPh3)2. Thus, the title compd. I (R = H, vinyl group substitution at 2 position; R1 = 4-Cl) was prepd.
IC ICM C07C211-45
ICS C07C211-56; C07C209-68
CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 68-12-2, uses 71-43-2, Benzene, uses **108-88-3**, Methylbenzene, uses **1330-20-7**, Dimethylbenzene, uses
RL: NUU (Other use, unclassified); USES (Uses)
(prepn. of 1-trifluoromethyl-2-alkylvinylaniline derivs.)
IT 106-47-8, reactions 127-08-2, Potassium acetate 127-09-3, Sodium acetate 144-55-8, Carbonic acid monosodium salt, reactions 298-14-6 338-75-0 431-21-0 497-19-8, Carbonic acid disodium salt, reactions 584-08-7 **688-74-4**, Tributoxyborane 1310-58-3, Potassium hydroxide (K(OH)), reactions 1310-73-2, Sodium hydroxide (Na(OH)), reactions 1514-82-5 2730-62-3 3282-30-2 7439-95-4, Magnesium, reactions 327165-13-9 327165-14-0 327165-15-1 327165-16-2
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(prepn. of 1-trifluoromethyl-2-alkylvinylaniline derivs.)
IT 65854-91-3P **185950-64-5P** 195372-65-7P 327165-11-7P 327165-12-8P

RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of 1-trifluoromethyl-2-alkylvinylaniline derivs.)

IT **108-88-3**, Methylbenzene, uses **1330-20-7**, Dimethylbenzene, uses
RL: NUU (Other use, unclassified); USES (Uses)
(prepn. of 1-trifluoromethyl-2-alkylvinylaniline derivs.)

RN 108-88-3 HCAPLUS
CN Benzene, methyl- (9CI) (CA INDEX NAME)

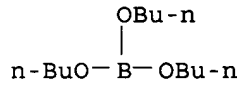


RN 1330-20-7 HCAPLUS
CN Benzene, dimethyl- (9CI) (CA INDEX NAME)

2 (D1—Me)

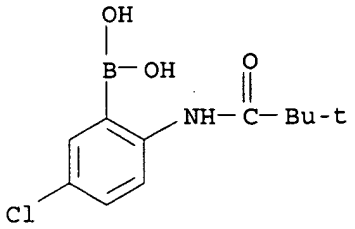
IT **688-74-4**, Tributoxyborane
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(prepn. of 1-trifluoromethyl-2-alkylvinylaniline derivs.)

RN 688-74-4 HCAPLUS
CN Boric acid (H3BO3), tributyl ester (8CI, 9CI) (CA INDEX NAME)



IT **185950-64-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of 1-trifluoromethyl-2-alkylvinylaniline derivs.)

RN 185950-64-5 HCAPLUS
CN Boronic acid, [5-chloro-2-[(2,2-dimethyl-1-oxopropyl)amino]phenyl]- (9CI) (CA INDEX NAME)



L35 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:96301 HCAPLUS
DOCUMENT NUMBER: 132:222614
TITLE: C2-Symmetric Planar Chiral Ferrocene Diamides by (-)-Sparteine-Mediated Directed ortho-**Lithiation**. Synthesis and Catalytic Activity
AUTHOR(S): Laufer, Radoslaw S.; Veith, Ulrich; Taylor, Nicholas J.; Snieckus, Victor
CORPORATE SOURCE: Guelph-Waterloo Centre for Graduate Work in Chemistry, University of Waterloo, Waterloo, ON, N2L 3G1, Can.
SOURCE: Organic Letters (2000), 2(5), 629-631
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:222614

AB A variety of highly enantioenriched singly and doubly functionalized derivs. of 1,1'-N,N,N',N'-tetraisopropylferrocenedicarboxamide were synthesized by (-)-sparteine-mediated directed ortho-metalation and Pd-catalyzed cross coupling reactions. The substituents at the 2 position were I, Me, Ph2COH, Et2COH, Bu3Sn, Ph2P, PhS, PhSe, and Me3Si. The synthetic applications of these chiral ligands in asym. alkylation of benzaldehyde by Et2Zn and Pd(0)-catalyzed allylic substitution of di-Me malonate by PhCH:CHCH(OAc)Ph or PhCH:CHCH(OH)Ph were demonstrated. Solvent-dependent enantiotopicity was obsd. for the asym. alkylation. The crystal and mol. structures of (S)-2-hydroxydiphenylmethyl-1,1'-N,N,N',N'-tetraisopropylferrocenedicarboxamide were detd. by x-ray crystallog.

CC 29-12 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22, 67, 75

ST crystal structure ferrocenedicarboxamide deriv enantiomer; mol structure ferrocenedicarboxamide deriv enantiomer; planar chiral ferrocene amide prepn ortho **lithiation** catalytic activity; asym alkylation catalyst planar chiral ferrocene amide; allylic substitution catalyst planar chiral ferrocene amide

IT Metallocenes
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(ferrocenes; synthesis and catalytic activity of C2-sym. planar chiral ferrocene diamides obtained by (-)-sparteine-mediated directed ortho-**lithiation**)

IT **Solvent** effect
(on enantiotopicity of alkylation of benzaldehyde by ethylzinc catalyzed by planar chiral ferrocenedicarboxamide deriv.)

IT **121-43-7**, Trimethyl borate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(condensation with dimethoxybromobenzene)

IT **133730-34-4P**, (2,4-Dimethoxyphenyl)boronic acid
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**

(Preparation); RACT (Reactant or reagent)
(**prepn**. and Suzuki cross coupling with planar chiral iodoferrocenedicarboxamide)

IT 191803-51-7P 261618-65-9P 261618-67-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and sparteine-mediated ortho-**lithiation** of)

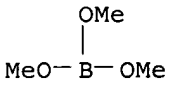
IT 107139-36-6P, 1,1'-N,N,N',N'-Tetraisopropylferrocenedicarboxamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and stereoselective ortho-**lithiation** mediated by sparteine enantiomer)

IT 75-77-4, Chlorotrimethylsilane, reactions 96-22-0, 3-Pentanone
119-61-9, Benzophenone, reactions 882-33-7, Diphenyl disulfide
1079-66-9, Diphenylphosphinous chloride 1461-22-9,
Tributyl(chloro)stannane 1666-13-3, Diphenyl diselenide
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with stereoselectively ortho-**lithiated** ferrocenedicarboxamide)

IT 90-39-1, (-)-Sparteine
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective ortho-**lithiation** of ferrocenedicarboxamide mediated by)

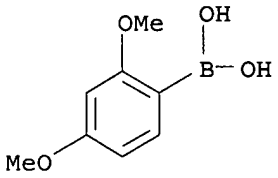
IT **121-43-7**, Trimethyl borate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(condensation with dimethoxybromobenzene)

RN 121-43-7 HCAPLUS
CN Boric acid (H3BO3), trimethyl ester (8CI, 9CI) (CA INDEX NAME)



IT **133730-34-4P**, (2,4-Dimethoxyphenyl)boronic acid
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(**prepn**. and Suzuki cross coupling with planar chiral iodoferrocenedicarboxamide)

RN 133730-34-4 HCAPLUS
CN Boronic acid, (2,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:629629 HCAPLUS
DOCUMENT NUMBER: 132:3224
TITLE: Highly Active Palladium Catalysts for Suzuki Coupling Reactions

AUTHOR(S): Wolfe, John P.; Singer, Robert A.; Yang, Bryant H.; Buchwald, Stephen L.
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SOURCE: Journal of the American Chemical Society (1999), 121(41), 9550-9561
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:3224

AB Mixts. of Pd(OAc)2 and o-(di-tert-butylphosphino)biphenyl catalyze the room-temp. Suzuki coupling of aryl bromides and aryl chlorides with 0.5-1.0 mol % Pd. Use of o-(dicyclohexylphosphino)biphenyl allows Suzuki couplings to be carried out at low catalyst loadings (0.000001-0.02 mol % Pd). The process tolerates a broad range of functional groups and substrate combinations including the use of sterically hindered substrates. This is the most active catalyst system in terms of reaction temp., turnover no., and steric tolerance which is reported to date.

CC 25-1 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT **89787-12-2P**, 2-Isopropylphenylboronic acid
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(**prepn**. and coupling with bromoiodobenzene)

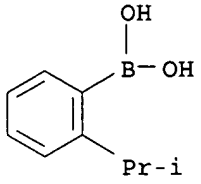
IT **5419-55-6**, Triisopropyl borate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction with bromoisopropylbenzene)

IT 95-46-5, 2-Bromotoluene 95-72-7, 1-Chloro-2,5-dimethylbenzene 98-80-6, Phenylboronic acid 99-90-1, Methyl 4-bromobenzoate 99-91-2 100-00-5, 4-Nitrophenyl chloride 103-88-8 106-41-2, 4-Bromophenol **106-43-4**, 4-Chlorotoluene 532-27-4, 2-Chloroacetophenone 553-94-6 576-22-7, 1-Bromo-2,6-dimethylbenzene 623-03-0, 4-Chlorobenzonitrile **623-12-1**, 4-Methoxyphenyl chloride 626-60-8, 3-Chloropyridine 766-51-8, 2-Chloroanisole 1003-09-4 1122-91-4, 4-Bromobenzaldehyde 1126-46-1, Methyl 4-chlorobenzoate 2856-63-5 3972-65-4, 4-tert-Butylphenyl bromide 5720-06-9 6781-98-2, 1-Chloro-2,6-dimethylbenzene 7051-16-3, 1-Chloro-3,5-dimethoxybenzene 17789-14-9 18982-54-2 22237-13-4 40138-16-7, 2-Formylphenylboronic acid 42371-64-2 100379-00-8, 2,6-Dimethylphenylboronic acid 204841-19-0 251320-80-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(room-temp. Suzuki coupling of aryl bromides or chlorides catalyzed by palladium acetate and phosphinobiphenyls)

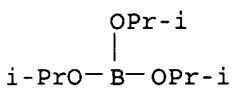
IT **89787-12-2P**, 2-Isopropylphenylboronic acid
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(**prepn**. and coupling with bromoiodobenzene)

RN 89787-12-2 HCAPLUS

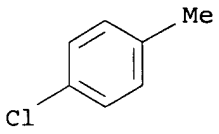
CN Boronic acid, [2-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



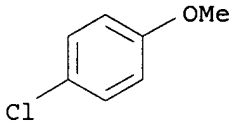
IT **5419-55-6**, Triisopropyl borate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction with bromoisopropylbenzene)
RN 5419-55-6 HCAPLUS
CN Boric acid (H3BO3), tris(1-methylethyl) ester (9CI) (CA INDEX NAME)



IT **106-43-4**, 4-Chlorotoluene **623-12-1**, 4-Methoxyphenyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(room-temp. Suzuki coupling of aryl bromides or chlorides catalyzed by palladium acetate and phosphinobiphenyls)
RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:543490 HCAPLUS
DOCUMENT NUMBER: 127:154946
TITLE: Difluorophenylpyrimidylpyridine derivatives and liquid-crystal mixtures and ferroelec. switching and/or display devices using them
INVENTOR(S): Nonaka, Toshiaki; Li, Ji; Takeichi, Ayako; Hornung, Barbara; Manero, Javier; Schmidt, Wolfgang; Wingen, Rainer
PATENT ASSIGNEE(S): Hoechst Aktiengesellschaft, Germany; Nonaka, Toshiaki; Li, Ji; Takeichi, Ayako; Hornung, Barbara; Manero, Javier; Schmidt, Wolfgang; Wingen, Rainer
SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9724351	A1	19970710	WO 1996-EP5774	19961220
W: CN, JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 09183973	A2	19970715	JP 1995-343288	19951228
DE 19648171	A1	19980528	DE 1996-19648171	19961121
EP 883618	A1	19981216	EP 1996-944617	19961220
EP 883618	B1	20010516		
R: DE, FR, GB				
JP 2000502688	T2	20000307	JP 1997-524013	19961220
US 6022492	A	20000208	US 1999-91404	19990114

PRIORITY APPLN. INFO.: JP 1995-343288 A 19951228
DE 1996-19648171 A 19961121
WO 1996-EP5774 W 19961220

OTHER SOURCE(S): MARPAT 127:154946

AB The invention relates to difluorophenylpyrimidylpyridine derivs. (I), where X = N and Y = CH or X = CH and Y = N; R1,R2 = (a) C1-20 alkyl in which (aa) .gtoreq.1 nonadjacent and nonterminal CH2 groups can be replaced by -O-, CO-O-, -O-CO-, -O-CO-O-, SiMe2-, and/or (ab) .gtoreq.1 H atoms can be replaced by F, and/or (ac) the terminal Me group can be replaced by 1 of the chiral groups II, III, R3CHCl-, R3CHF-, R3CH(CN)-, R3CH(CH3)-, R3CHFCHF- (optically active or racemic); or (b) H, where only one of the radicals R1, R2 may be H, provided that R1 may not be bonded to the pyridine ring by means of -CO-O- or -O-CO-O-; R3,R4,R5 = H or C1-16 alkyl (with or without an asym. C atom), in which .gtoreq.1 nonadjacent, nonterminal CH2 groups can be replaced by -O-, and/or .gtoreq.1 H atoms of the alkyl radical can be substituted by F; R4 and R5 can also be -(CH2)4- or -(CH2)5- together, when they are bound to a dioxolane system. The derivs. are particularly suitable as constituents in ferroelec. liq.-crystal mixts. for display devices.

IC ICM C07D405-04
ICS C09K019-34; C09K019-58; C07D405-14

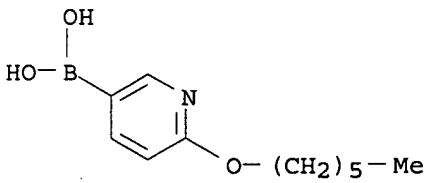
CC 75-11 (Crystallography and Liquid Crystals)
Section cross-reference(s): 28, 74

IT 134321-89-4P 154115-63-6P 155802-44-1P **193400-05-4P**
193400-06-5P 193400-07-6P 193400-08-7P 193400-09-8P 193400-10-1P
193400-11-2P 193400-12-3P 193400-13-4P 193400-14-5P 193400-15-6P
193400-16-7P 193400-17-8P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(**prepn**. and reaction of; in synthesis of difluorophenylpyrimidylpyridine derivs. for liq.-crystal mixts. and display devices)

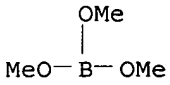
IT 74-83-9, Bromomethane, reactions 109-65-9, 1-Bromobutane 111-14-8, Heptanoic acid 111-25-1, 1-Bromohexane 111-27-3, 1-Hexanol, reactions 111-83-1, 1-Bromooctane **121-43-7 121-44-8**, reactions 541-41-3 624-28-2, 2,5-Dibromopyridine 32779-36-5, 5-Bromo-2-chloropyrimidine 32779-37-6, 2,5-Dibromopyrimidine 97275-47-3, (1S,2S)-1-Butyl-2-(hydroxymethyl)oxirane 121219-16-7 121219-22-5 127608-48-4 144933-29-9 147223-09-4 147223-24-3 156635-87-9 193400-34-9 193400-35-0
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction of; in synthesis of difluorophenylpyrimidylpyridine derivs. for liq.-crystal mixts. and display devices)

IT **193400-05-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(**prepn**. and reaction of; in synthesis of

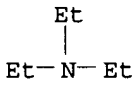
difluorophenylpyrimidylpyridine derivs. for liq.-crystal mixts. and display devices)
RN 193400-05-4 HCAPLUS
CN Boronic acid, [6-(hexyloxy)-3-pyridinyl]- (9CI) (CA INDEX NAME)



IT **121-43-7 121-44-8**, reactions
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(reaction of; in synthesis of difluorophenylpyrimidylpyridine derivs. for liq.-crystal mixts. and display devices)
RN 121-43-7 HCAPLUS
CN Boric acid (H3BO3), trimethyl ester (8CI, 9CI) (CA INDEX NAME)



RN 121-44-8 HCAPLUS
CN Ethanamine, N,N-diethyl- (9CI) (CA INDEX NAME)



L35 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:227816 HCAPLUS
DOCUMENT NUMBER: 122:45681
TITLE: The synthesis and biological activity of tetrahydroquinoline angiotensin II antagonists containing a substituted biphenyltetrazole group
AUTHOR(S): Thomas, Andrew P.; Roberts, David A.; Thomason, Douglas A.
CORPORATE SOURCE: ZENECA Pharmaceuticals, Cheshire, SK10 4TG, UK
SOURCE: Bioorganic & Medicinal Chemistry Letters (1994), 4(21), 2615-20
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:45681
AB The synthesis of analogs of tetrahydroquinoline angiotensin II antagonists, ZENECA ZD6888, bearing substituents on the biphenyl ring system is reported. Several of these compds. show comparable or superior activity to ZD6888 in an in vitro binding assay and in inhibition of the angiotensin II-induced pressor response in normotensive rats.
CC 1-3 (Pharmacology)

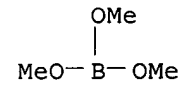
Section cross-reference(s): 27, 28

IT **121-43-7**, Trimethyl borate **121-44-8**, reactions
589-15-1 813-19-4 2042-37-7 5720-05-8, p-Tolylboronic acid
17846-68-3, Tributyltin azide 42872-83-3 76283-09-5 138642-33-8
138642-36-1 138642-39-4 138642-47-4 138642-60-1 138642-63-4
160013-17-2 160013-18-3 160013-24-1
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(synthesis and biol. activity of tetrahydroquinoline angiotensin II receptor antagonists contg. substituted biphenyltetrazole group in relation to antihypertensive activity)

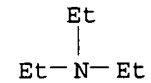
IT **68162-47-0P** 138620-94-7P 138620-95-8P 138620-96-9P
138642-59-8P 138642-61-2P **138642-62-3P** 138642-64-5P
140221-62-1P **143805-55-4P** 160013-15-0P 160013-25-2P
160013-26-3P 160013-27-4P 160013-28-5P 160013-29-6P 160013-30-9P
160013-34-3P 161205-20-5P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(synthesis and biol. activity of tetrahydroquinoline angiotensin II receptor antagonists contg. substituted biphenyltetrazole group in relation to antihypertensive activity)

IT **121-43-7**, Trimethyl borate **121-44-8**, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(synthesis and biol. activity of tetrahydroquinoline angiotensin II receptor antagonists contg. substituted biphenyltetrazole group in relation to antihypertensive activity)

RN 121-43-7 HCAPLUS
CN Boric acid (H3BO3), trimethyl ester (8CI, 9CI) (CA INDEX NAME)

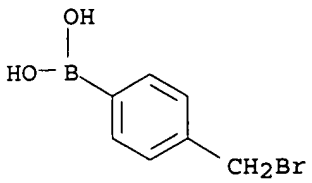


RN 121-44-8 HCAPLUS
CN Ethanamine, N,N-diethyl- (9CI) (CA INDEX NAME)

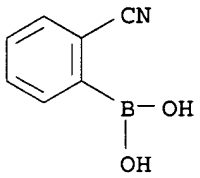


IT **68162-47-0P 138642-62-3P 143805-55-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(synthesis and biol. activity of tetrahydroquinoline angiotensin II receptor antagonists contg. substituted biphenyltetrazole group in relation to antihypertensive activity)

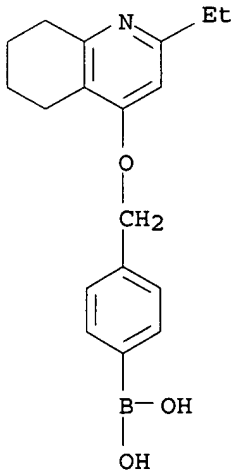
RN 68162-47-0 HCAPLUS
CN Boronic acid, [4-(bromomethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 138642-62-3 HCAPLUS
CN Boronic acid, (2-cyanophenyl)- (9CI) (CA INDEX NAME)



RN 143805-55-4 HCAPLUS
CN Boronic acid, [4-[[(2-ethyl-5,6,7,8-tetrahydro-4-quinolinyl)oxy]methyl]phenyl]- (9CI) (CA INDEX NAME)



L35 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1994:631530 HCAPLUS
DOCUMENT NUMBER: 121:231530
TITLE: Rigid-rod polyelectrolytes: synthesis of sulfonated poly(p-phenylene)s
AUTHOR(S): Rulkens, Rudy; Schulze, Margit; Wegner, Gerhard
CORPORATE SOURCE: Max-Planck-Inst. Polymerforsch., Mainz, D-55128, Germany
SOURCE: Macromolecular Rapid Communications (1994), 15(9), 669-76
CODEN: MRCOE3; ISSN: 1022-1336
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Copolymer precursors of 3-methylphenyl 2,5-dibromobenzenesulfonate with 2-dodecyl-5-methyl-1,4-benzenediboronic acid 1,3-propanediol ester or 2,5-dihexyl-1,4-benzenediboronic acid (I) and of I with 2,2'-bis(4-methylbenzenesulfonato)-4,4'-dibromobiphenyl were prepd. by polycondensation, characterized by NMR, and converted to the title polymers by hydrolysis. The liq. cryst. properties of the title polymers wer studied.

CC 35-5 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 75

IT 106-37-6, 1,4-Dibromobenzene 106-38-7, 4-Bromotoluene **106-43-4**, 4-Chlorotoluene **121-43-7**, Trimethyl borate 143-15-7, Dodecyl bromide 504-63-2, 1,3-Propanediol
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(in prepn. of sulfonated poly(p-phenylene)s rigid-rod polyelectrolytes)

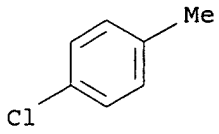
IT 104-41-6P 158153-85-6P **158153-86-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(in **prepn**. of sulfonated poly(p-phenylene)s rigid-rod polyelectrolytes)

IT **5720-05-8P**, (4-Methylbenzene)boronic acid
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(in **prepn**. of sulfonated poly(p-phenylene)s rigid-rod polyelectrolytes)

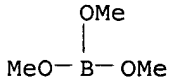
IT 158153-92-5DP, hydrolyzed 158153-92-5P **158153-93-6P** **158153-95-8P** 158153-96-9P 158343-61-4P 158343-62-5DP, hydrolyzed 158343-62-5P
RL: PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**
(**prepn**. and liq. cryst. properties of rigid polyelectrolyte poly(p-phenylene)s)

IT **106-43-4**, 4-Chlorotoluene **121-43-7**, Trimethyl borate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(in prepn. of sulfonated poly(p-phenylene)s rigid-rod polyelectrolytes)

RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



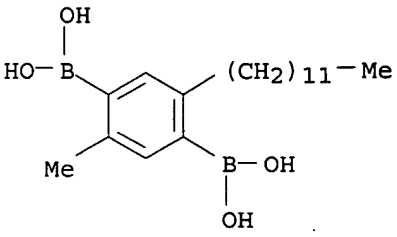
RN 121-43-7 HCAPLUS
CN Boric acid (H3BO3), trimethyl ester (8CI, 9CI) (CA INDEX NAME)



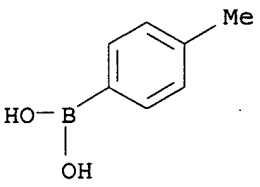
IT **158153-86-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(in **prepn**. of sulfonated poly(p-phenylene)s rigid-rod polyelectrolytes)

RN 158153-86-7 HCAPLUS
CN Boronic acid, (2-dodecyl-5-methyl-1,4-phenylene)bis- (9CI) (CA INDEX

NAME)



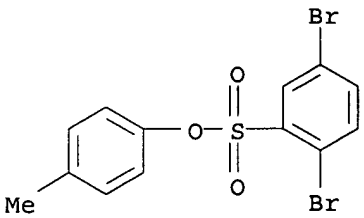
IT **5720-05-8P**, (4-Methylbenzene)boronic acid
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(in **prepn**. of sulfonated poly(p-phenylene)s rigid-rod polyelectrolytes)
RN 5720-05-8 HCAPLUS
CN Boronic acid, (4-methylphenyl)- (9CI) (CA INDEX NAME)



IT **158153-93-6P 158153-95-8P**
RL: PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**
(**prepn**. and liq. cryst. properties of rigid polyelectrolyte poly(p-phenylene)s)
RN 158153-93-6 HCAPLUS
CN Benzenesulfonic acid, 2,5-dibromo-, 4-methylphenyl ester, polymer with (2,5-dihexyl-1,4-phenylene)bis[boronic acid] (9CI) (CA INDEX NAME)

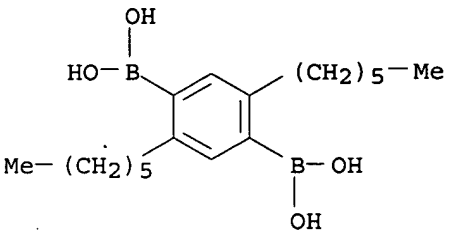
CM 1

CRN 158153-89-0
CMF C13 H10 Br2 O3 S



CM 2

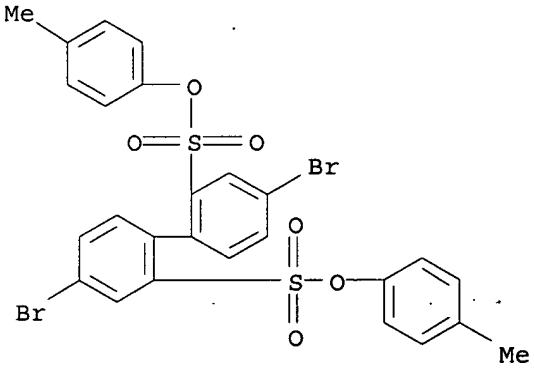
CRN 131117-66-3
CMF C18 H32 B2 O4



RN 158153-95-8 HCAPLUS
CN [1,1'-Biphenyl]-2,2'-disulfonic acid, 4,4'-dibromo-, bis(4-methylphenyl) ester, polymer with (2,5-dihexyl-1,4-phenylene)bis[boronic acid] (9CI) (CA INDEX NAME)

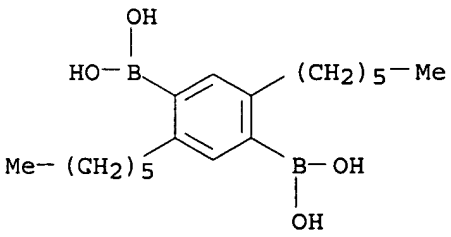
CM 1

CRN 158153-94-7
CMF C26 H20 Br2 O6 S2



CM 2

CRN 131117-66-3
CMF C18 H32 B2 O4



L35 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1994:534130 HCAPLUS
DOCUMENT NUMBER: 121:134130
TITLE: Process for the preparation of phenyltetrazole

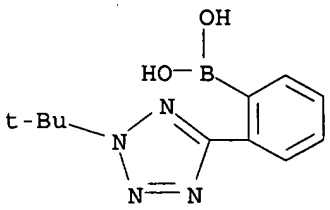
derivatives azo organoboron intermediates
INVENTOR(S): Chekroun, Isaac; Ruiz Montes, Jose; Bedoya Zurita, Manuel; Rossey, Guy
PATENT ASSIGNEE(S): Synthelabo S. A., Fr.
SOURCE: Fr. Demande, 11 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2696745	A1	19940415	FR 1992-12167	19921012
FR 2696745	B1	19950512		

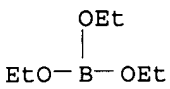
OTHER SOURCE(S): CASREACT 121:134130; MARPAT 121:134130

AB The title compds. [I; A = (un)substituted aryl, (un)substituted heterocyclyl; R1-R3 = C1-2 alkyl, aryl] are prepd. in high yields by the reaction of benzeneboronic acids II with organohalides AZ (Z = halogen) in the presence of Na2CO3 and Pd[P(Ph)3]4. Thus, [2-[2-(1,1-dimethylethyl)-2H-tetrazol-5-yl]phenyl]boronic acid was reacted with 1-bromonaphthalene in the presence of Na2CO3 and Pd[P(Ph)3]4, producing 2-(1,1-dimethylethyl)-5-[2-(1-naphthyl)phenyl]-2H-tetrazole, m.p. 83-85.degree., in 57% yield.

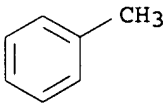
IC ICM C07D401-10
ICS C07D257-04; C07D403-10; C07D471-04
ICI C07D401-10, C07D213-58, C07D257-04; C07D403-10, C07D239-30, C07D257-04; C07D401-10, C07D215-12, C07D257-04; C07D471-04, C07D213-74, C07D233-64
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 29
IT **151512-28-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(**prepn**. and reaction of, in **prepn**. of phenylteterazole derivs.)
IT 90-11-9 **150-46-9**, Triethyl borate 612-62-4, 2-Chloroquinoline 626-55-1, 3-Bromopyridine 3934-20-1, 2,4-Dichloropyrimidine 4295-11-8, 2-Chloro-6-methylquinoline 154466-54-3, 2-(1,1-Dimethylethyl-5-(2-iodophenyl)-2H-tetrazole 157101-22-9
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction of, in prepn. of phenylteterazole derivs.)
IT **108-88-3**, Toluene, uses
RL: RCT (Reactant); RACT (Reactant or reagent)
(solvent, in prepn. of phenyltetrazole derivs.)
IT **151512-28-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(**prepn**. and reaction of, in **prepn**. of phenylteterazole derivs.)
RN 151512-28-6 HCAPLUS
CN Boronic acid, [2-[2-(1,1-dimethylethyl)-2H-tetrazol-5-yl]phenyl]- (9CI) (CA INDEX NAME)



IT **150-46-9**, Triethyl borate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction of, in prepn. of phenylteterazole derivs.)
RN 150-46-9 HCAPLUS
CN Boric acid (H3BO3), triethyl ester (8CI, 9CI) (CA INDEX NAME)



IT **108-88-3**, Toluene, uses
RL: RCT (Reactant); RACT (Reactant or reagent)
(solvent, in prepn. of phenyltetrazole derivs.)
RN 108-88-3 HCAPLUS
CN Benzene, methyl- (9CI) (CA INDEX NAME)



L35 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1993:671389 HCAPLUS
DOCUMENT NUMBER: 119:271389
TITLE: Tetrazolylphenylboronic acid intermediates for the synthesis of angiotensin II receptor antagonists
INVENTOR(S): Lo, Young Sek; Rossano, Lucius Thomas; Larsen, Robert D.; King, Anthony O.
PATENT ASSIGNEE(S): du Pont de Nemours, E. I., and Co., USA; Merck and Co., Inc.
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9310106	A1	19930527	WO 1992-US9979	19921118
W: AU, CA, CS, FI, JP, KR, NO, PL				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, SE				
US 5130439	A	19920714	US 1991-793514	19911118
US 5206374	A	19930427	US 1992-911813	19920710

US 5310928	A	19940510	US 1992-911812	19920710
AU 9331792	A1	19930615	AU 1993-31792	19921118
AU 665388	B2	19960104		
EP 643704	A1	19950322	EP 1993-900550	19921118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, SE				
JP 08500323	T2	19960116	JP 1992-509518	19921118
PL 171453	B1	19970430	PL 1992-303787	19921118
PL 176124	B1	19990430	PL 1992-312131	19921118
SK 280887	B6	20000912	SK 1994-579	19921118
FI 9402282	A	19940517	FI 1994-2282	19940517
NO 9401857	A	19940718	NO 1994-1857	19940518

PRIORITY APPLN. INFO.: US 1991-793514 A 19911118
US 1992-911812 A 19920710
US 1992-911813 A 19920710
WO 1992-US9979 A 19921118

OTHER SOURCE(S): CASREACT 119:271389; MARPAT 119:271389

AB Title compds. I [P = Ph3C, Me3C, C1-4-alkoxymethyl, MeSCH2, Ph-C1-4-alkoxymethyl, p-MeOC6H4CH2, 2,4,6-trimethylbenzyl, 2-(trimethylsilyl)ethyl, tetrahydropyranyl, piperonyl, benzenesulfonyl; R1a, R1b = independently Cl, Br, C1-4-alkoxy, OH; or R1aBR1b = II, A = Ph (sic) or (CH2)n, n = 2-4] were prepd. as intermediates for the synthesis of angiotensin II receptor antagonists. Thus, reaction of B(OCHMe2)3 with the Li salt of 5-phenyl-2-trityltetrazole carbanion (generated from 5-phenyl-2-trityltetrazole and BuLi), followed by AcOH/H2O hydrolysis, afforded title compd. I (P = 2'-Ph3C, R1a = R1b= OH) (III). More advanced intermediates that are precursors for angiotensin II receptor antagonists are prepd. by cross-coupling of I with QC6H4X [X = Br, I, methanesulfonyloxy, toluenesulfonyloxy, fluorosulfonyloxy, trifluoromethanesulfonyloxy; Q = H, Me, C1-4-alkyl, hydroxymethyl, triorganosiloxymethyl, hydroxy-C1-4-alkyl, formyl, C1-4-acyl, C1-4-alkoxycarbonyl, WL [L = single bond, (CH2)t, t = 1-4, (CH2)rO(CH2)r, (CH2)rSOr(CH2)r, r = 0-2] and W = IV (R2 = C1-4-alkyl, Y = e.g., C1-4-alkyl, Z = e.g., hydroxymethyl)] in presence of metal catalyst, base, and coupling solvent to afford biphenyls V. Coupling of III with QC6H4X [X = 4-Br; Q = WL [L = CH2, W = IV (R2 = Bu, Y = Cl, Z = CH2OH)]] with catalyst formed from Pd chloride, Ph3P, and P(OCHMe2)3 afforded the corresponding V in 90% yield.

IC ICM C07D257-02

CC 29-4 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 1, 28

IT **121-44-8**, Triethylamine, uses 122-08-7 497-19-8, Carbonic acid disodium salt, uses 534-17-8, Cesium carbonate 584-08-7, Potassium carbonate 2052-49-5, Tetrabutylammonium hydroxide 7087-68-5, Diisopropylethylamine 12026-06-1, Thallium hydroxide 26628-22-8, Sodium azide (Na(N3))
RL: RCT (Reactant); RACT (Reactant or reagent)
(base, for prepn. of angiotensin II receptor antagonist intermediates)

IT **5419-55-6**, Triisopropyl borate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(boration reaction with, in prepn. of angiotensin II receptor antagonist intermediates)

IT **143722-25-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(**prepn.** and coupling reaction of, in **prepn.** angiotensin II receptor antagonist intermediates)

IT 114798-26-4P 124750-99-8P **143722-30-9P** **143722-31-0P** 150097-93-1P 151012-30-5P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(**prepn.** of, as angiotensin II receptor antagonist

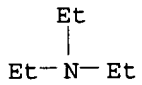
intermediate)

IT 108-10-1, Methyl isobutyl ketone
RL: RCT (Reactant); RACT (Reactant or reagent)
(recrystn. **solvent**, for prepn. of angiotensin II receptor antagonist intermediates)

IT **60-29-7**, Diethyl ether, uses 64-17-5, Ethanol, uses 67-56-1, Methanol, uses 67-68-5, uses 68-12-2, DMF, uses 71-23-8, Propanol, uses 71-43-2, Benzene, uses 75-05-8, Acetonitrile, uses 96-47-9, 2-Methyltetrahydrofuran **108-88-3**, Toluene, uses **109-99-9**, uses 123-91-1, 1,4-Dioxane, uses 127-19-5, Dimethylacetamide 462-95-3, Diethoxymethane 7732-18-5, Water, uses
RL: RCT (Reactant); RACT (Reactant or reagent)
(**solvent**, for prepn. of angiotensin II receptor antagonist intermediates)

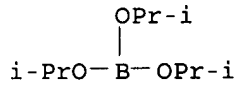
IT **121-44-8**, Triethylamine, uses
RL: RCT (Reactant); RACT (Reactant or reagent)
(base, for prepn. of angiotensin II receptor antagonist intermediates)

RN 121-44-8 HCAPLUS
CN Ethanamine, N,N-diethyl- (9CI) (CA INDEX NAME)



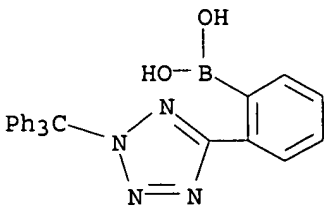
IT **5419-55-6**, Triisopropyl borate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(boration reaction with, in prepn. of angiotensin II receptor antagonist intermediates)

RN 5419-55-6 HCAPLUS
CN Boric acid (H3BO3), tris(1-methylethyl) ester (9CI) (CA INDEX NAME)



IT **143722-25-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(**prepn.** and coupling reaction of, in **prepn.** angiotensin II receptor antagonist intermediates)

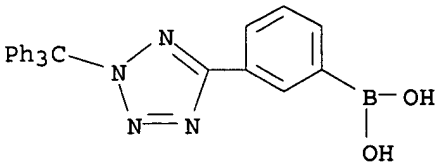
RN 143722-25-2 HCAPLUS
CN Boronic acid, [2-[2-(triphenylmethyl)-2H-tetrazol-5-yl]phenyl]- (9CI) (CA INDEX NAME)



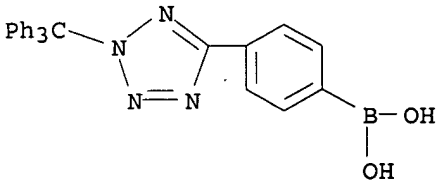
IT **143722-30-9P 143722-31-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**

(**prepn**. of, as angiotensin II receptor antagonist intermediate)

RN 143722-30-9 HCAPLUS
CN Boronic acid, [3-[2-(triphenylmethyl)-2H-tetrazol-5-yl]phenyl]- (9CI) (CA INDEX NAME)

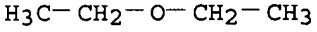


RN 143722-31-0 HCAPLUS
CN Boronic acid, [4-[2-(triphenylmethyl)-2H-tetrazol-5-yl]phenyl]- (9CI) (CA INDEX NAME)

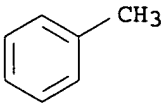


IT **60-29-7**, Diethyl ether, uses **108-88-3**, Toluene, uses **109-99-9**, uses
RL: RCT (Reactant); RACT (Reactant or reagent)
(**solvent**, for prepn. of angiotensin II receptor antagonist intermediates)

RN 60-29-7 HCAPLUS
CN Ethane, 1,1'-oxybis- (9CI) (CA INDEX NAME)



RN 108-88-3 HCAPLUS
CN Benzene, methyl- (9CI) (CA INDEX NAME)

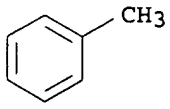


RN 109-99-9 HCAPLUS
CN Furan, tetrahydro- (7CI, 8CI, 9CI) (CA INDEX NAME)

L35 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1987:496769 HCAPLUS
DOCUMENT NUMBER: 107:96769
TITLE: Flash vacuum pyrolysis of o-alkylaryl- and arylalkylchloroboranes. Synthesis of benzoannulated boracycloalkenes
AUTHOR(S): Schacht, Wolfgang; Kaufmann, Dieter
CORPORATE SOURCE: Inst. Org. Chem., Univ. Hamburg, Hamburg, D-2000/13, Fed. Rep. Ger.
SOURCE: Chem. Ber. (1987), 120(8), 1331-8
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 107:96769

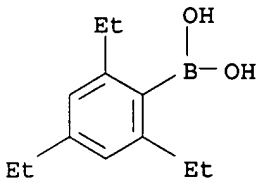
AB 2,4,6-R3C6H2BCl2 (I; R = Me, Et) were prepd. by the reaction of triorganoboroxins or aryltrimethylsilanes with BCl3. 2-R1C6H4BCl2 (II; R1 = Et, Pr, CHMe2) and 2-R2C6H4(CH2)nBCl2 (III; R2 = H, Me; n = 1, 2) were prepd. by the reaction of tetraorganostannanes with BCl3. Flash vacuum pyrolysis of I (R = Et) and II (R1 = Et) gave boraindans IV (R3 = H, Et; R4, R5 = H). I (R = Me) and II (R1 = Me) were completely stable on pyrolysis. Pyrolysis of II (R1 = CHMe2) gave IV (R3, R5 = H, R4 = Me), whereas pyrolysis of II (R1 = Pr) gave mixt. of IV (R3, R4 = H, R5 = Me) and boratetralin (V). Pyrolysis of III (R2 = Me, n = 1) gave exclusively 2-chloro-2-boraindan. At 950.degree., pyrolysis of III (R2 = H, n = 1) gave benzoborete dimer (VI). The inversion barrier of IV was .DELTA.G228 = 10.3 kcal/mol, detd. by NMR. Similarly, pyrolysis of III (R2 = H, Me; n = 2) gave mixts. of boraindan analogs and (PhCH2CH2)2BCl or (2-MeC6H4CH2CH2)2BCl.

CC 29-4 (Organometallic and Organometalloidal Compounds)
IT 95-49-8P, 2-Chlorotoluene **108-88-3P**, Toluene, preparation
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by pyrolysis of dichlorotolylborane)
IT **108593-75-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**
(**prepn**. and thermolysis of)
IT **121-43-7**, Trimethoxyborane
RL: **RCT (Reactant)**
(reaction of, with (triethyl)phenyl Grignard reagent)
IT **10294-34-5**, Trichloroborane
RL: **RCT (Reactant)**
(ring cleavage by, of tris(trialkylphenyl)boroxins)
IT **108-88-3P**, Toluene, preparation
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by pyrolysis of dichlorotolylborane)
RN 108-88-3 HCAPLUS
CN Benzene, methyl- (9CI) (CA INDEX NAME)

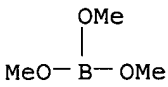


IT **108593-75-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**
(**prepn**. and thermolysis of)

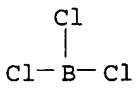
RN 108593-75-5 HCAPLUS
CN Boronic acid, (2,4,6-triethylphenyl)- (9CI) (CA INDEX NAME)



IT **121-43-7**, Trimethoxyborane
RL: **RCT (Reactant)**
(reaction of, with (triethyl)phenyl Grignard reagent)
RN 121-43-7 HCAPLUS
CN Boric acid (H3BO3), trimethyl ester (8CI, 9CI) (CA INDEX NAME)

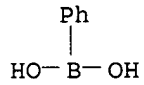


IT **10294-34-5**, Trichloroborane
RL: **RCT (Reactant)**
(ring cleavage by, of tris(trialkylphenyl)boroxins)
RN 10294-34-5 HCAPLUS
CN Borane, trichloro- (9CI) (CA INDEX NAME)

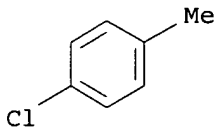


L36 ANSWER 1 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:531853 HCAPLUS
DOCUMENT NUMBER: 137:232594
TITLE: Facile Synthesis of N-Alkyl-N'-arylimidazolium Salts via Addition of Imidazoles to Arynes
AUTHOR(S): Yoshida, Hiroto; Sugiura, Shinji; Kunai, Atsutaka
CORPORATE SOURCE: Department of Applied Chemistry Graduate School of Engineering, Hiroshima University, Higashi-Hiroshima, 739-8527, Japan
SOURCE: Organic Letters (2002), 4(16), 2767-2769
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A novel synthetic approach to N-alkyl-N'-arylimidazolium salts has been developed on the basis of addn. of imidazoles to arynes. A variety of N-alkyl-N'-arylimidazolium salts can be synthesized straightforwardly in modest to good yields. Furthermore, the utility of the resulting imidazolium salts has been demonstrated by the palladium-catalyzed

Suzuki-Miyaura coupling of aryl chlorides.
CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
IT **98-80-6**, Phenylboronic acid 99-91-2, 4'-Chloroacetophenone **106-43-4**, p-Chlorotoluene 616-47-7, 1-Methylimidazole 1739-84-0, 1,2-Dimethylimidazole 3475-07-8, 1-Methyl-2-phenylimidazole 4238-71-5, 1-Benzylimidazole 4316-42-1, 1-Butylimidazole 4532-96-1, 1-Isopropylimidazole 20075-26-7, 1-(Methoxymethyl)imidazole 45676-04-8, 1-tert-Butylimidazole 88284-48-4 217813-03-1 252054-91-4 458566-99-9 458567-00-5 458567-01-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of N-alkyl-N'-arylimidazolium salts via addn. of imidazoles to arynes)
IT **98-80-6**, Phenylboronic acid **106-43-4**, p-Chlorotoluene
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of N-alkyl-N'-arylimidazolium salts via addn. of imidazoles to arynes)
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:525771 HCAPLUS
DOCUMENT NUMBER: 137:216710
TITLE: Highly Active Oxime-Derived Palladacycle Complexes for Suzuki-Miyaura and Ullmann-Type Coupling Reactions
AUTHOR(S): Alonso, Diego A.; Najera, Carmen; Pacheco, M. Carmen
CORPORATE SOURCE: Departamento de Quimica Organica, Universidad de Alicante, Alicante, 03080, Spain
SOURCE: Journal of Organic Chemistry (2002), 67(16), 5588-5594
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Oxime-derived chloro-bridged palladacycles I (R1 = H, Cl, MeO), II, and III are efficient complexes for the Suzuki-Miyaura reactions of aryl-, allyl-, and benzyl halides with arylboronic acids. These catalysts are thermally stable, not sensitive to air or moisture, and easily accessible from inexpensive starting materials. The Suzuki-Miyaura reactions can be performed under aerobic conditions with aryl bromides and chlorides, displaying turnover nos. (TON) of up to 5 .times. 105 and turnover frequencies (TOF) of up to 198 000 h-1 for aryl bromides, and TON of up to

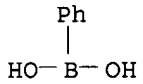
4700 and TOF up to 4700 h-1 for aryl chlorides. Even inexpensive and readily available benzyl and allyl chlorides underwent the coupling reaction with good turnover nos. I (R1 = Cl) also catalyzed the reductive coupling of iodoarenes giving the corresponding sym. biaryls in good yields.

CC 25-2 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

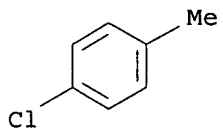
IT 90-11-9, 1-Bromonaphthalene 92-66-0, 4-Bromobiphenyl **98-80-6**, Phenylboronic acid 99-90-1 99-91-2 104-92-7, 4-Bromoanisole 106-41-2, 4-Bromophenol **106-43-4**, 4-Chlorotoluene 623-03-0, 4-Chlorobenzonitrile **623-12-1**, 4-Chloroanisole 626-60-8, 3-Chloropyridine 780-20-1 873-32-5, 2-Chlorobenzonitrile 933-76-6 1450-75-5, Ethanone, 1-(5-bromo-2-hydroxyphenyl)- 1878-68-8, 4-Bromophenylacetic acid 2042-37-7, 2-Bromobenzonitrile 4701-17-1, 5-Bromo-2-thiophenecarboxaldehyde **5720-05-8**, (4-Methylphenyl)boronic acid 6940-50-7 10602-01-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biaryls via Suzuki-Miyaura coupling of aryl bromides and chlorides with phenylboronic acids catalyzed by oxime-derived palladacycle complexes)

IT **98-80-6**, Phenylboronic acid **106-43-4**, 4-Chlorotoluene **623-12-1**, 4-Chloroanisole **5720-05-8**, (4-Methylphenyl)boronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biaryls via Suzuki-Miyaura coupling of aryl bromides and chlorides with phenylboronic acids catalyzed by oxime-derived palladacycle complexes)

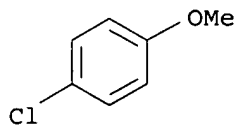
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



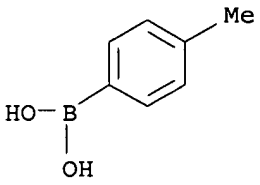
RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



RN 5720-05-8 HCAPLUS
CN Boronic acid, (4-methylphenyl)- (9CI) (CA INDEX NAME)

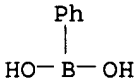


REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

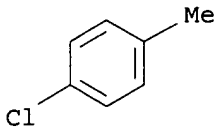
L36 ANSWER 3 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:516202 HCAPLUS
DOCUMENT NUMBER: 137:79086
TITLE: Preparation of carbene diene complexes of nickel, palladium, and platinum as catalysts for Heck or coupling reactions
INVENTOR(S): Beller, Matthias; Andreo, Mario Gomez; Zapf, Alexander; Karch, Ralf; Kleinwaechter, Ingo; Briel, Oliver
PATENT ASSIGNEE(S): OMG Ag & Co. Kg, Germany
SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10062577	A1	20020711	DE 2000-10062577	20001215

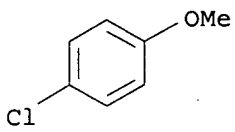
OTHER SOURCE(S): CASREACT 137:79086; MARPAT 137:79086
AB The invention concerns carbene diene complexes of nickel, palladium, and platinum, e.g. I, and its use as catalysts in org.-chem. reactions. Thus, carbene complex I catalyzed Heck reaction of 4-ClC6H4Me with PhCH:CH2 gave 35% 4-MeC6H4CH:CHPh, whereas, similar I catalyzed coupling reaction of 4-ClC6H4F with phenylboronic acid gave 45% 4-PhC6H4F.
IC ICM C07F015-00
ICS C07F015-04; B01J031-12
CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 25
IT 74-85-1, Ethene, reactions **98-80-6** 100-42-5, Styrene, reactions 103-11-7 **106-43-4**, 4-Chlorotoluene 108-90-7, Chlorobenzene, reactions 111-34-2 141-32-2 348-51-6, 1-Chloro-2-fluorobenzene 352-33-0, 1-Chloro-4-fluorobenzene **623-12-1**, 4-Chloroanisole 626-60-8, 3-Chloropyridine 873-32-5, 2-Chlorobenzonitrile 5111-65-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of carbene diene complexes of nickel, palladium, and platinum as catalysts for Heck or coupling reactions)
IT **98-80-6** **106-43-4**, 4-Chlorotoluene **623-12-1**, 4-Chloroanisole
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of carbene diene complexes of nickel, palladium, and platinum as catalysts for Heck or coupling reactions)
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 4 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:509541 HCAPLUS
DOCUMENT NUMBER: 137:217039
TITLE: Air Stable, Sterically Hindered Ferrocenyl Dialkylphosphines for Palladium-Catalyzed C-C, C-N, and C-O Bond-Forming Cross-Couplings
AUTHOR(S): Kataoka, Noriyasu; Shelby, Quinetta; Stambuli, James P.; Hartwig, John F.
CORPORATE SOURCE: Dep. Chem., Yale Univ., New Haven, CT, 06520-8107, USA
SOURCE: Journal of Organic Chemistry (2002), 67(16), 5553-5566
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Pentaphenylferrocenyl di-tert-butylphosphine I (R = R1 = Ph) was prepd.; the scope of various cross-coupling processes catalyzed by palladium complexes of I has been investigated. I (R = R1 = Ph) was prepd. by lithiation of ferrocene followed by removal of solvent, addn. of a 5:1 pentane:THF mixt., and addn. of di(tert-butyl)chlorophosphine to give mono(di-tert-butylphosphino)ferrocene with high chemoselectivity; arylation of the ferrocenylphosphine with chlorobenzene as a solvent in the presence of palladium (II) acetate and sodium tert-butoxide yielded I in 40-65% yield overall. I (R = R1 = Ph) acts as a highly effective ligand for palladium-catalyzed amination and for Suzuki coupling reactions with aryl- and alkylboronic acids. Unactivated, electron-rich, and electron-poor aryl bromides and chlorides undergo coupling reactions in the presence of palladium complexes of I (R = R1 = Ph) with high turnover nos. Aryl bromides were coupled to alcs. in the presence of I (R = R1 = Ph); silanols and electron-rich phenols were coupled to activated aryl

halides in the presence of I (R = R1 = Ph). Intramol. coupling reactions of alcs. and aryl bromides were successful, although substrates with hydrogens .alpha. to the alc. oxygen underwent some .beta.-hydride elimination. Acyclic and cyclic primary and secondary alkyl- and arylamines underwent coupling reactions with aryl bromides and chlorides in the presence of I (R = R1 = Ph). Aryl- and primary alkylboronic acids underwent coupling reactions in the presence of I (R = R1 = Ph); coupling of alkylboronic acids with aryl halides was successful in the absence of toxic or expensive bases. Other substituted ferrocenylphosphines I (R = R1 = 4-MeOC6H4, 4-F3CC6H4) were prepd. but palladium catalysts derived from the ligands showed little difference in catalytic activity when compared to palladium catalysts derived from I (R = R1 = Ph). Palladium catalysts derived from I (R = R1 = 3,5-Me2C6H3) were active in coupling reactions with aryl halides and alcs. but not in amination or Suzuki coupling reactions; I (R = Ph; R1 = H) acted as a catalyst for coupling reactions but gave significantly decreased yields due to decreased steric hindrance of the reaction center in the palladium complexes. I (R = R1 = Ph) not only generates highly active palladium catalysts, but is also air stable both in soln. and in the solid state. Palladium(0) complexes of I (R = R1 = Ph) are air stable solids and react only slowly with oxygen in soln. Crystal structure of I (R = R1 = Ph; R = Ph; R1 = H) were detd. by X-ray crystallog.

CC 29-12 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 25, 75

IT **98-80-6**, Phenylboronic acid **1679-18-1**, 4-Chlorophenylboronic acid **5720-07-0**, 4-Methoxyphenylboronic acid 13922-41-3, 1-Naphthylboronic acid **16419-60-6**, 2-Methylphenylboronic acid **87199-17-5**, 4-Formylphenylboronic acid **128796-39-4**, 4-(Trifluoromethyl)phenylboronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of arenes by coupling reactions of aryl boronic acids with aryl bromides and chlorides in the presence of palladium complexes of a (pentaphenylferrocenyl)di(tert-butyl)phosphine)

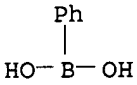
IT 90-11-9, 1-Bromonaphthalene 90-90-4, 4-Bromobenzophenone 95-46-5, 2-Bromotoluene 95-49-8, 2-Chlorotoluene 95-72-7, 2-Chloro-p-xylene 100-00-5, 1-Chloro-4-nitrobenzene 104-88-1, 4-Chlorobenzaldehyde, reactions 104-92-7, 4-Bromoanisole 106-38-7, 4-Bromotoluene **106-43-4**, 4-Chlorotoluene 108-86-1, Bromobenzene, reactions 134-85-0, 4-Chlorobenzophenone 553-94-6, 2-Bromo-p-xylene 576-22-7, 2-Bromo-m-xylene 578-57-4, 2-Bromoanisole 586-78-7, 1-Bromo-4-nitrobenzene 591-17-3, 3-Bromotoluene 623-00-7, 4-Bromobenzonitrile 623-03-0, 4-Chlorobenzonitrile 694-80-4, 1-Bromo-2-chlorobenzene 766-51-8, 2-Chloroanisole 1122-91-4, 4-Bromobenzaldehyde 1126-46-1, Methyl 4-chlorobenzoate 2398-37-0, 3-Bromoanisole 2635-13-4, 5-Bromo-1,3-benzodioxole 2845-89-8, 3-Chloroanisole 3972-65-4, 1-Bromo-4-tert-butylbenzene 6781-98-2, 2-Chloro-m-xylene 19393-92-1, 2-Bromo-1,3-dichlorobenzene 64380-53-6, 2-(3-Chlorophenyl)-1,3-dioxolane
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of aryl amines, aryl ethers, and arenes by palladium-catalyzed amination, substitution, and Suzuki coupling reactions of aryl halides in the presence of a (pentaphenylferrocenyl)di(tert-butyl)phosphine)

IT 98-56-6, 1-Chloro-4-(trifluoromethyl)benzene 102-54-5, Ferrocene 108-90-7, Chlorobenzene, reactions 556-96-7, 5-Bromo-m-xylene **623-12-1**, p-Chloroanisole 4045-44-7, 1,2,3,4,5-Pentamethylcyclopentadiene 13716-10-4, Chlorodi(tert-butyl)phosphine 76181-95-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pentaarylferrocenylphosphines as air-stable ligands for palladium-catalyzed amination and Suzuki coupling reactions with aryl

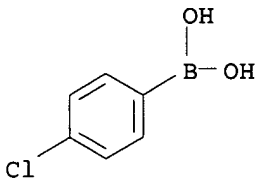
chlorides and bromides)

IT **98-80-6**, Phenylboronic acid **1679-18-1**, 4-Chlorophenylboronic acid **5720-07-0**, 4-Methoxyphenylboronic acid **16419-60-6**, 2-Methylphenylboronic acid **87199-17-5**, 4-Formylphenylboronic acid **128796-39-4**, 4-(Trifluoromethyl)phenylboronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn.** of arenes by coupling reactions of aryl boronic acids with aryl bromides and chlorides in the presence of palladium complexes of a (pentaphenylferrocenyl)di(tert-butyl)phosphine)

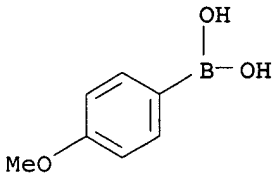
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



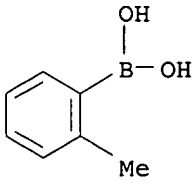
RN 1679-18-1 HCAPLUS
CN Boronic acid, (4-chlorophenyl)- (9CI) (CA INDEX NAME)



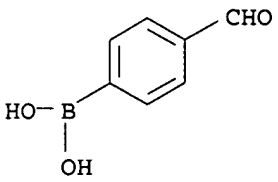
RN 5720-07-0 HCAPLUS
CN Boronic acid, (4-methoxyphenyl)- (9CI) (CA INDEX NAME)



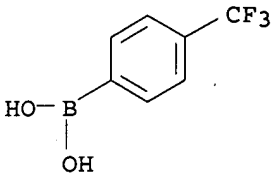
RN 16419-60-6 HCAPLUS
CN Boronic acid, (2-methylphenyl)- (9CI) (CA INDEX NAME)



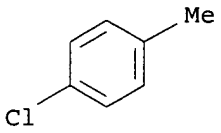
RN 87199-17-5 HCAPLUS
CN Boronic acid, (4-formylphenyl)- (9CI) (CA INDEX NAME)



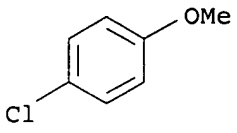
RN 128796-39-4 HCAPLUS
CN Boronic acid, [4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



IT **106-43-4**, 4-Chlorotoluene
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of aryl amines, aryl ethers, and arenes by palladium-catalyzed amination, substitution, and Suzuki coupling reactions of aryl halides in the presence of a (pentaphenylferrocenyl)di(tert-butyl)phosphine)
RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



IT **623-12-1**, p-Chloroanisole
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of pentaarylferrocenylphosphines as air-stable ligands for palladium-catalyzed amination and Suzuki coupling reactions with aryl chlorides and bromides)
RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 82 THERE ARE 82 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 5 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:466019 HCAPLUS
DOCUMENT NUMBER: 137:33413
TITLE: Preparation of sterically hindered phosphine ligands

and their use as cocatalyst in Heck reaction
INVENTOR(S): Hartwig, John F.; Stambuli, James; Stauffer, Shaun R.
PATENT ASSIGNEE(S): Yale University, USA
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002048160	A1	20020620	WO 2001-US47853	20011211

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

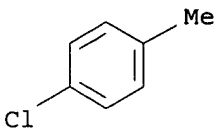
PRIORITY APPLN. INFO.: US 2000-255057P P 20001212
US 2001-13156 A 20011210
OTHER SOURCE(S): CASREACT 137:33413; MARPAT 137:33413

AB The present invention is directed to a catalyst compn., comprising a Group 8 metal; and a ligand P{C(CH2R)(CH2R1)(CH2R2)}3 (R, R1, R2 = H, C1-10 organoalkoxy, diorganoamino) or P(CMe3)(Ad)(L) (Ad = adamantyl, C1-30 hydrocarbyl). The present invention is also directed to a method of forming carbon-carbon, carbon-oxygen, carbon-sulfur, and carbon-nitrogen bonds between substrates using the above catalysts. Thus, CuI/LiBr/THF/Et2O mediated phosphination of 1,1-dimethylpropylmagnesium chloride with PCl3 gave 40.5% tris(1,1-dimethylpropyl)phosphine which was used as cocatalyst in Pd(dba)2 catalyzed Heck arylation vinyl substrates.

IC ICM C07F009-50
ICS C07F015-00; C07F015-02; C07F015-04; C07F015-06; C07C211-43
CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 25
IT 96-33-3, Methyl acrylate 100-42-5, Styrene, reactions 100-46-9, Benzylamine, reactions 100-61-8, reactions 104-92-7, 4-Bromoanisole **106-43-4**, p-Chlorotoluene 106-49-0, reactions 108-86-1, Bromobenzene, reactions 110-91-8, Morpholine, reactions 111-26-2, Hexyl amine 111-86-4, Octylamine 122-39-4, Diphenylamine, reactions 141-32-2, Butyl acrylate 578-57-4, 2-Bromoanisole 3972-65-4, 4-tert-Butylbromobenzene 26915-12-8, Tolylamine 41492-05-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of sterically hindered phosphine ligands as cocatalyst in palladium catalyzed Heck arylation reaction)
IT **98-80-6**, Phenylboronic acid 100-59-4, Phenylmagnesium chloride 693-03-8, Butylmagnesium bromide **1679-18-1**, 4-Chlorophenylboronic acid **5720-05-8** **5720-06-9**, o-Methoxyphenylboronic acid **5720-07-0**, p-Methoxyphenylboronic acid 13922-41-3, 1-Naphthylboronic acid **16419-60-6**, o-Tolylboronic acid 28557-00-8, Phenylzinc chloride 42930-39-2, Butylzinc chloride 74133-06-5 **87199-17-5**, 4-Formylphenylboronic acid **128796-39-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of sterically hindered phosphine ligands as cocatalyst in palladium catalyzed bond formation reaction)
IT **106-43-4**, p-Chlorotoluene

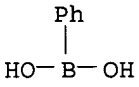
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of sterically hindered phosphine ligands as cocatalyst in palladium catalyzed Heck arylation reaction)

RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)

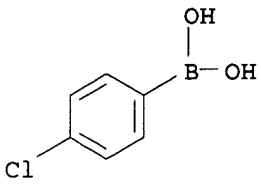


IT **98-80-6**, Phenylboronic acid **1679-18-1**, 4-Chlorophenylboronic acid **5720-05-8** **5720-06-9**, o-Methoxyphenylboronic acid **5720-07-0**, p-Methoxyphenylboronic acid **16419-60-6**, o-Tolylboronic acid **87199-17-5**, 4-Formylphenylboronic acid **128796-39-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of sterically hindered phosphine ligands as cocatalyst in palladium catalyzed bond formation reaction)

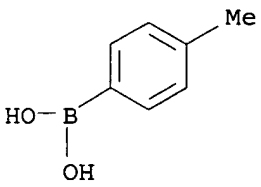
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



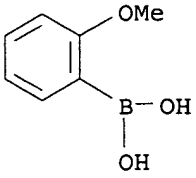
RN 1679-18-1 HCAPLUS
CN Boronic acid, (4-chlorophenyl)- (9CI) (CA INDEX NAME)



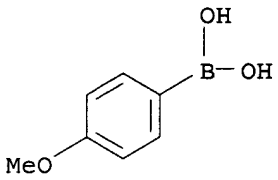
RN 5720-05-8 HCAPLUS
CN Boronic acid, (4-methylphenyl)- (9CI) (CA INDEX NAME)



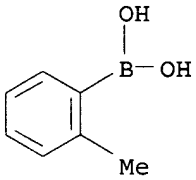
RN 5720-06-9 HCAPLUS
CN Boronic acid, (2-methoxyphenyl)- (9CI) (CA INDEX NAME)



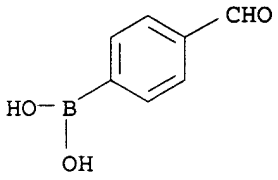
RN 5720-07-0 HCAPLUS
CN Boronic acid, (4-methoxyphenyl)- (9CI) (CA INDEX NAME)



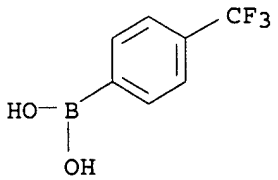
RN 16419-60-6 HCAPLUS
CN Boronic acid, (2-methylphenyl)- (9CI) (CA INDEX NAME)



RN 87199-17-5 HCAPLUS
CN Boronic acid, (4-formylphenyl)- (9CI) (CA INDEX NAME)



RN 128796-39-4 HCAPLUS
CN Boronic acid, [4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 6 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:385668 HCAPLUS
TITLE: Combinatorial libraries with P-functionalized aminopyridines: ligands for the preparation of efficient C(aryl)-Cl activation catalysts
AUTHOR(S): Schareina, Thomas; Kempe, Rhett
CORPORATE SOURCE: Institut fur Organische Katalyseforschung, Rostock, 18055, Germany
SOURCE: Angewandte Chemie, International Edition (2002), 41(9), 1521-1523
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The parallel synthesis of homogeneous catalysts is successful with ligands such as P,P-diphenyl-N,N-di-2-pyridinylphosphinous amide. They coordinate metals of Group 10 with the formation of a five-membered chelate ring, e.g., dichloro(P,P-diphenyl-N,N-di-2-pyridinylphosphinous amide-NN,P)palladium. The resulting metal complexes are efficient catalysts which can activate C(aryl)-chloro bonds and can, for example, mediate the Suzuki coupling of 3-chloropyridine with phenylboronic acid to form 3-phenylpyridine.

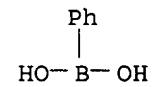
CC 25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 75

IT INDEXING IN PROGRESS

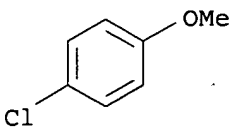
IT **98-80-6**, Phenylboronic acid 623-03-0, 4-Chlorobenzonitrile **623-12-1**, 1-Chloro-4-methoxybenzene 626-60-8, 3-Chloropyridine 1079-66-9, Diphenylphosphinous chloride 1202-34-2 3140-73-6, 2-Chloro-4,6-dimethoxy-1,3,5-triazine 12107-56-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(ligands for **prepn**. of C(aryl)-chloro activation catalysts [dichloro(P,P-diaryl-N,N-bis(pyridinyl))phosphinous amide-NN,P)palladium analogs and derivs.])

IT **98-80-6**, Phenylboronic acid **623-12-1**, 1-Chloro-4-methoxybenzene
RL: RCT (Reactant); RACT (Reactant or reagent)
(ligands for **prepn**. of C(aryl)-chloro activation catalysts [dichloro(P,P-diaryl-N,N-bis(pyridinyl))phosphinous amide-NN,P)palladium analogs and derivs.])

RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 7 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:323890 HCAPLUS
DOCUMENT NUMBER: 137:140613
TITLE: N-heterocyclic carbenes. Part 32. A defined N-heterocyclic carbene complex for the palladium-catalyzed Suzuki cross-coupling of aryl chlorides at ambient temperatures
AUTHOR(S): Gstottmayr, Christian W. K.; Bohm, Volker P. W.; Herdtweck, Eberhardt; Grosche, Manja; Herrmann, Wolfgang A.
CORPORATE SOURCE: Anorganisch-chemisches Institut Technische Universitat Munchen, Garching, 85747, Germany
SOURCE: Angewandte Chemie, International Edition (2002), 41(8), 1363-1365
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:140613

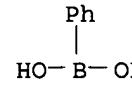
AB Suzuki cross-coupling of aryl chlorides is possible with a palladium(0) complex bearing two bulky, N-heterocyclic carbene ligands. Nearly quant. yields are obtained within two hours with some reagents, which makes this compd. the most active catalyst known to date under these conditions. Thus, reaction of Pd(PBut3)2 with 1,3-bis(adamantyl)imidazolin-2-ylidene in hexane gave 83% palladium carbene complex I (Ad = adamantyl) which was used as catalyst for Suzuki cross-coupling reaction of 4-MeC6H4Cl with PhB(OH)2 in dioxane to give 97% 4-MeC6H4Ph.

CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 25, 75

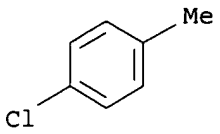
IT 98-56-6, 1-Chloro-4-(trifluoromethyl)benzene **98-80-6**, Phenylboronic acid 99-91-2 **106-43-4**, 4-Tolyl chloride 108-41-8, 1-Chloro-3-methylbenzene **623-12-1**, 4-Chloroanisole **10365-98-7**, 3-Methoxyphenylboronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of sterically demanding imidazolinylidene palladium carbene complex as catalyst Suzuki cross-coupling of aryl chlorides with arylboronic acids at ambient temps.)

IT **98-80-6**, Phenylboronic acid **106-43-4**, 4-Tolyl chloride **623-12-1**, 4-Chloroanisole **10365-98-7**, 3-Methoxyphenylboronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of sterically demanding imidazolinylidene palladium carbene complex as catalyst Suzuki cross-coupling of aryl chlorides with arylboronic acids at ambient temps.)

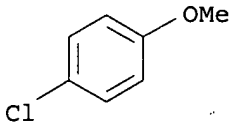
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



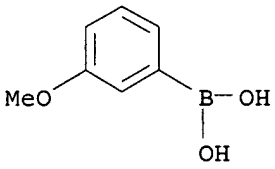
RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



RN 10365-98-7 HCAPLUS
CN Boronic acid, (3-methoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 8 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:886941 HCAPLUS
DOCUMENT NUMBER: 136:167119
TITLE: Palladium-Catalyzed Three-Component Assembling of Allenes, Organic Halides, and Arylboronic Acids
AUTHOR(S): Huang, Tai-Hsiang; Chang, Hao-Ming; Wu, Ming-Yuan; Cheng, Chien-Hong
CORPORATE SOURCE: Department of Chemistry, Tsing Hua University, Hsinchu, Taiwan
SOURCE: Journal of Organic Chemistry (2002), 67(1), 99-105
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:167119
AB An efficient method for the construction of two carbon-carbon bonds in a regio- and stereoselective fashion via palladium-catalyzed assembling of allenes, org. halides, and arylboronic acids is described. Org. halides (RI = PhI, o-, m-, and p-MeOC6H4I, p-EtO2CC6H4I, p-AcC6H4I, p-MeC6H4I, p-MeC6H4Br, p-MeC6H4Cl, p-NO2C6H4I, p-NO2C6H4Br, p-NO2C6H4Cl, p-IC6H4Cl, 1-iodonaphthalene, 2-iodothiophene, 3-iodo-2-cyclopenten-1-one, 3-iodo-5,5-dimethyl-2-cyclohexen-1-one, PhCBr:CH2 and ICH2CO2Et), and arylboronic acids [ArB(OH)2; Ar = Ph, p-MeOC6H4, m-NO2C6H4, p-FC6H4, 1-naphthyl, o-, m-, and p-(OCH)C6H4] undergo Suzuki-type three-component assembling with 1,1-dimethylallene to give allylic derivs., Me2:CRCH2Ar, in DMF at 70.degree. in the presence of CsF and Pd(dba)2 as the catalyst. Higher yields of products were obtained for aryl iodides than for the

corresponding aryl bromides and chlorides. This three-component assembling is highly regioselective, with the org. group on halides adding to the middle carbon and the aryl group on arylboronic acids to the unsubstituted terminal carbon of allenes. Monosubstituted allenes (cyclopentylallene, cyclohexylallene, tert-butylallene, and n-butylallene) also undergo similar assembling reaction with org. halides and arylboronic acids to afford the corresponding products with high regio- and stereoselectivity. Based on the known palladium chem., a mechanism is proposed to account for the catalytic reaction and the stereochem.

CC 25-2 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

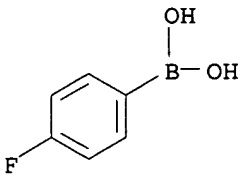
IT **1765-93-1**, (4-Fluorophenyl)boronic acid **5720-07-0**, (4-Methoxyphenyl)boronic acid **13331-27-6**, (3-Nitrophenyl)boronic acid 13922-41-3, 1-Naphthaleneboronic acid **40138-16-7**, (2-Formylphenyl)boronic acid **87199-16-4**, (3-Formylphenyl)boronic acid **87199-17-5**, (4-Formylphenyl)boronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of diarylmethylbutenes via Pd-catalyzed, regioselective three-component condensation of dimethylallene, org. halides, and arylboronic acids)

IT 90-14-2, 1-Iodonaphthalene **98-80-6**, Phenylboronic acid 98-81-7, .alpha.-Bromostyrene 100-00-5, 4-Chloronitrobenzene 106-38-7, 4-Bromotoluene **106-43-4**, 4-Chlorotoluene 529-28-2, 2-Iodoanisole 586-78-7, 4-Bromonitrobenzene 591-50-4, Iodobenzene 598-25-4, 1,1-Dimethylallene 623-48-3, Ethyl iodoacetate 624-31-7, 4-Iodotoluene 636-98-6, 4-Iodonitrobenzene 637-87-6, 4-Iodochlorobenzene 696-62-8, 4-Iodoanisole 766-85-8, 3-Iodoanisole 3437-95-4, 2-Iodothiophene 13329-40-3, 4-Iodoacetophenone 51934-41-9, Ethyl 4-iodobenzoate 56671-85-3 61765-46-6, 3-Iodo-2-cyclopenten-1-one
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of diarylmethylbutenes via Pd-catalyzed, regioselective three-component condensation of dimethylallene, org. halides, and phenylboronic acid)

IT **1765-93-1**, (4-Fluorophenyl)boronic acid **5720-07-0**, (4-Methoxyphenyl)boronic acid **13331-27-6**, (3-Nitrophenyl)boronic acid **40138-16-7**, (2-Formylphenyl)boronic acid **87199-16-4**, (3-Formylphenyl)boronic acid **87199-17-5**, (4-Formylphenyl)boronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of diarylmethylbutenes via Pd-catalyzed, regioselective three-component condensation of dimethylallene, org. halides, and arylboronic acids)

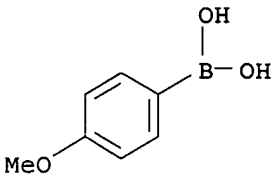
RN 1765-93-1 HCAPLUS

CN Boronic acid, (4-fluorophenyl)- (9CI) (CA INDEX NAME)

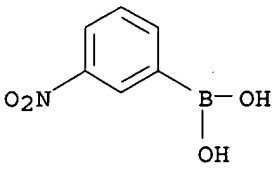


RN 5720-07-0 HCAPLUS

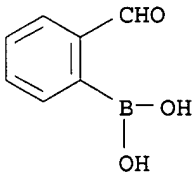
CN Boronic acid, (4-methoxyphenyl)- (9CI) (CA INDEX NAME)



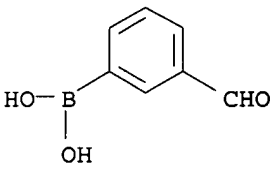
RN 13331-27-6 HCAPLUS
CN Boronic acid, (3-nitrophenyl)- (9CI) (CA INDEX NAME)



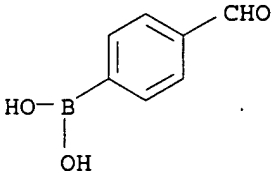
RN 40138-16-7 HCAPLUS
CN Boronic acid, (2-formylphenyl)- (9CI) (CA INDEX NAME)



RN 87199-16-4 HCAPLUS
CN Boronic acid, (3-formylphenyl)- (9CI) (CA INDEX NAME)



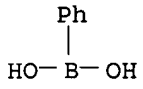
RN 87199-17-5 HCAPLUS
CN Boronic acid, (4-formylphenyl)- (9CI) (CA INDEX NAME)



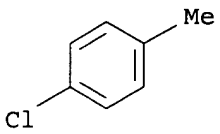
IT **98-80-6**, Phenylboronic acid **106-43-4**, 4-Chlorotoluene
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of diarylmethylbutenes via Pd-catalyzed,

regioselective three-component condensation of dimethylallene, org. halides, and phenylboronic acid)

RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 9 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:772171 HCAPLUS
DOCUMENT NUMBER: 135:318588
TITLE: Biaryl phosphine and amine ligands for improved transition metal-catalyzed processes
INVENTOR(S): Buchwald, Stephen L.; Old, David W.; Wolfe, John P.; Palucki, Michael; Kamikawa, Ken
PATENT ASSIGNEE(S): Massachusetts Institute of Technology, USA
SOURCE: U.S., 55 pp., Cont.-in-part of U.S. Ser. No. 113,478. CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6307087	B1	20011023	US 1999-231315	19990113
US 6395916	B1	20020528	US 1998-113478	19980710
CA 2336691	AA	20000120	CA 1999-2336691	19990709
WO 2000002887	A2	20000120	WO 1999-US15450	19990709
WO 2000002887	A3	20000629		
W: CA, JP				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1097158	A2	20010509	EP 1999-933785	19990709
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002520328	T2	20020709	JP 2000-559117	19990709

PRIORITY APPLN. INFO.:
US 1998-113478 A2 19980710
US 1998-196855 A 19981120
US 1999-231315 A 19990113
US 1999-239024 A 19990127
WO 1999-US15450 W 19990709

OTHER SOURCE(S): CASREACT 135:318588; MARPAT 135:318588

AB The present invention relates to the prepn. of novel biaryl phosphine and amine ligands (I) [wherein A and B = independently fused monocyclic or polycyclic cycloalkyl, cycloalkenyl, aryl, or heterocyclic rings of 4-8 atoms; X = NR2, PR2, AsR2, OR, or SR; Y = NR2, PR2, AsR2, OR, SR, SiR3, alkyl, or H; R-R6 = independently H, halogen, (hetero)alkyl, alkenyl, alkynyl, hydroxy, alkoxy, silyloxy, amino, nitro, sulfhydryl, amide, carbonyl, ketone, anhydride, silyl, thioalkyl, ketone, ester, nitrile, (hetero)aryl, etc.] for transition metals and their use in metal-catalyzed carbon-heteroatom and carbon-carbon bond-forming reactions. Unexpected improvements over the prior art were demonstrated in transition metal-catalyzed aryl amination reactions, Suzuki couplings giving both biaryl and alkylaryl products, arylations and vinylations at the position .alpha. to carbonyl groups, and carbon-oxygen bond formation. The ligands and methods of the invention enable transformations utilizing aryl chlorides and bromides at room temp. at synthetically useful rates with extremely small amts. of catalyst relative to the limiting reagent. For example, coupling of p-chlorobenzonitrile and morpholine was catalyzed by 2.5 mol% Pd2(dba)3, 7.5 mol% of 2-(N,N-dimethylamino)-2'-(dicyclohexylphosphino)biphenyl, and NaOBu-t in DME at room temp. to provide 4-(4-morpholinyl)benzonitrile in 96% yield. Thus, the subject processes provide improvements in many features of the transition metal-catalyzed reactions, including the range of suitable substrates, reaction conditions, and efficiency.

IC ICM C07C255-03
ICS C07F009-28; C07D265-30; C07D211-70; C07D209-04

NCL 558388000

CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 25

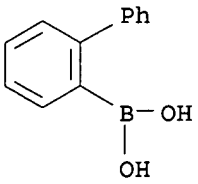
IT **4688-76-0P** 20837-12-1P 59734-92-8P 75295-57-7P
89291-23-6P 128796-39-4P, 4-(Trifluoromethyl)phenylboronic acid 157282-19-4P 213697-67-7P 224311-57-3P 224311-58-4P 224311-59-5P 255837-15-1P, 2-Bromo-4'(trifluoromethyl)biphenyl 255837-16-2P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)

IT 95-72-7 98-80-6 99-90-1 99-91-2 100-00-5, 1-Chloro-4-nitrobenzene 100-46-9, Benzylamine, reactions 100-61-8, n-Methylaniline, reactions 103-88-8, 4'-Bromoacetanilide 106-38-7 106-41-2, 4-Bromophenol **106-43-4** 106-49-0, p-Toluidine, reactions 108-94-1, Cyclohexanone, reactions 110-91-8, Morpholine, reactions 111-26-2, Hexylamine 111-92-2, Dibutylamine 120-72-9, Indole, reactions 123-75-1, Pyrrolidine, reactions 402-43-7, 4-(Trifluoromethyl)phenyl bromide 460-00-4, 1-Bromo-4-fluorobenzene 553-94-6, 2-Bromo-p-xylene 556-96-7 563-80-4 565-69-5 576-22-7 583-53-9, 1,2-Dibromobenzene 583-55-1, 2-Bromoiodobenzene 592-41-6, 1-Hexene, reactions 619-42-1 623-03-0, 4-Chlorobenzonitrile **623-12-1** 626-60-8, 3-Chloropyridine 698-00-0 768-90-1, 1-Bromoadamantane 1003-09-4, 2-Bromothiophene 1013-88-3, Benzophenone imine 1079-66-9, Chlorodiphenylphosphine 1122-91-4, 4-Bromobenzaldehyde 1126-46-1 2052-07-5, 2-Bromobiphenyl 2142-68-9, 2'-Chloroacetophenone 2856-63-5, 2-Chlorobenzyl cyanide 3972-65-4, 1-Bromo-4-t-butylbenzene 5720-06-9 7051-16-3 13716-10-4, Chlorodi-tert-butylphosphine 16523-54-9, Chlorodicyclohexylphosphine 17933-03-8 18982-54-2, 2-Bromobenzylalcohol 22237-13-4, 4-Ethoxyphenylboronic acid 40138-16-7 42371-64-2 53847-33-9 74866-28-7, 2,2'-Dibromo-1,1'-binaphthyl 204841-19-0, 3-Acetylphenyl boronic acid 251320-89-5, 2-(Bromo)-2'-(isopropyl)biphenyl
RL: RCT (Reactant); RACT (Reactant or reagent)

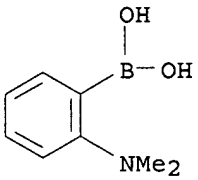
(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)

IT **4688-76-0P 89291-23-6P 128796-39-4P,** 4-(Trifluoromethyl)phenylboronic acid
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)

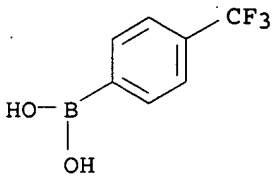
RN 4688-76-0 HCAPLUS
CN Boronic acid, [1,1'-biphenyl]-2-yl- (9CI) (CA INDEX NAME)



RN 89291-23-6 HCAPLUS
CN Boronic acid, [2-(dimethylamino)phenyl]- (9CI) (CA INDEX NAME)

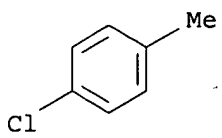


RN 128796-39-4 HCAPLUS
CN Boronic acid, [4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

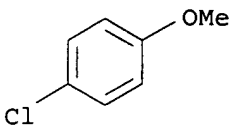


IT **106-43-4 623-12-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(biaryl phosphine and amine ligands for improved transition metal-catalyzed processes)

RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)

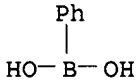


RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)

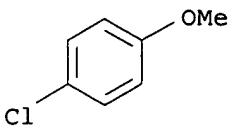


REFERENCE COUNT: 131 THERE ARE 131 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 10 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:603089 HCAPLUS
DOCUMENT NUMBER: 136:5513
TITLE: Highly active catalysts for the Suzuki coupling of aryl chlorides
AUTHOR(S): Bedford, Robin B.; Cazin, Catherine S. J.
CORPORATE SOURCE: School of Chemistry, University of Exeter, Exeter, EX4 4QD, UK
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2001), (17), 1540-1541
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Simple tricyclohexylphosphine adducts of palladium complexes with orthometalated N-donor ligands show by far the highest activity yet reported in the Suzuki coupling of aryl chlorides, even under aerobic conditions. Thus, [2-[(dimethylamino-.kappa.N)methyl]phenyl-.kappa.C](tricyclohexylphosphine)(trifluoroacetato-.kappa.O)palladium was easily prepd. from a corresponding dimeric precursor and tricyclohexylphosphine.
CC 21-2 (General Organic Chemistry)
IT 95-49-8, 2-Chlorotoluene **98-80-6**, Phenylboronic acid 99-91-2 100-00-5, 4-Chloronitrobenzene 104-88-1, 4-Chlorobenzaldehyde, reactions **623-12-1**, 4-Chloroanisole 766-51-8, 2-Chloroanisole 2622-14-2, Tricyclohexylphosphine
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of [[(dimethylamino-.kappa.N)methyl]phenyl-.kappa.C](cyclohexylphosphine)(trifluoroacetato)palladium derivs. as Suzuki coupling catalysts for aryl chlorides)
IT **98-80-6**, Phenylboronic acid **623-12-1**, 4-Chloroanisole
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of [[(dimethylamino-.kappa.N)methyl]phenyl-.kappa.C](cyclohexylphosphine)(trifluoroacetato)palladium derivs. as Suzuki coupling catalysts for aryl chlorides)
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)

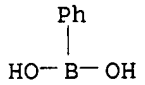


RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)

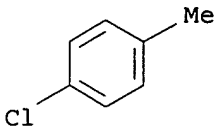


REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

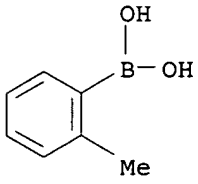
L36 ANSWER 11 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:372470 HCAPLUS
DOCUMENT NUMBER: 135:180850
TITLE: Synthesis of a C3-symmetric ferrocenylphosphine and its application to the Suzuki reaction of aryl chlorides
AUTHOR(S): Pickett, T. E.; Richards, C. J.
CORPORATE SOURCE: Department of Chemistry, Cardiff University, Cardiff, CF10 3TB, UK
SOURCE: Tetrahedron Letters (2001), 42(22), 3767-3769
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:180850
AB (pS,pS,pS)-Tris(2-methylferrocenyl)phosphine was synthesized in 62% yield from (S)-2-ferrocenyl-4-(1-methylethyl)-2-oxazoline. In combination with Pd2dba3, this novel C3-sym. ligand generates a catalyst for the Suzuki reaction of aryl chloride substrates, these reactions proceeding readily at 60.degree. in dioxane.
CC 29-12 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 25
IT 95-49-8, o-Chlorotoluene **98-80-6**, Phenylboronic acid 100-00-5, 1-Chloro-4-nitrobenzene **106-43-4**, p-Chlorotoluene 108-90-7, Chlorobenzene, reactions 766-51-8, 2-Chloroanisole **16419-60-6**, o-Tolylboronic acid 162157-03-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of C3-sym. ferrocenylphosphine and its application to Suzuki reaction of aryl chlorides)
IT **98-80-6**, Phenylboronic acid **106-43-4**, p-Chlorotoluene **16419-60-6**, o-Tolylboronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of C3-sym. ferrocenylphosphine and its application to Suzuki reaction of aryl chlorides)
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



RN 16419-60-6 HCAPLUS
CN Boronic acid, (2-methylphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 12 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:785819 HCAPLUS
DOCUMENT NUMBER: 133:335334
TITLE: Preparation of palladium and nickel complexes of biphenyl-2-yl-phosphines and their application in catalytic carbon-carbon, carbon-nitrogen, and carbon-oxygen coupling reactions
INVENTOR(S): Haber, Steffen; Meudt, Andreas; Noerenberg, Antje; Scherer, Stefan; Vollmueller, Frank
PATENT ASSIGNEE(S): Clariant G.m.b.H., Germany
SOURCE: Ger. Offen., 14 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19920847	A1	20001109	DE 1999-19920847	19990506
WO 2000068237	A1	20001116	WO 2000-EP3710	20000426

W: BR, CA, CN, IL, JP, KR, MX
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

PRIORITY APPLN. INFO.: DE 1999-19920847 A 19990506
OTHER SOURCE(S): MARPAT 133:335334
AB The invention concerns the prepn. of new Pd and Ni-complexes of biphenyl-2-yl-phosphines I (R1, R2 = same or different straight chain or branched C1-8 alkyl, C4-8 cycloalkyl, C2-12 alkenyl, C2-12 alkynyl, (un)substituted Ph, hetero aryl; R1R2 = C3-8 1,.omega.-alkanediyl chain; R3 = H, C1-12 alkyl, C2-12 alkenyl, C2-12 alkynyl, Ph, Naphthyl, hetero aryl, Li, Na, K, MgCl, MgBr, MgI, Mg0.5, ZnCl, ZnBr, Zn0.5, POPhenyl2, PO-(C1-C8-alkyl)2, PO3-(C1-C8-alkyl)2, SO2R, SOR, SiR3, C(:O)R, C(:O)NR2, C(:O)NHR, C(:O)OR; or R3 = a polymer matrix, which is connected to neighboring phenolic oxygen atom directly or by an aliph., arom. or araliph. bridge member with the R3; R4-R11 = H, org. substituent). The

new complexes can be used as catalysts for C-C-, C-N-, and C-O-coupling, e.g. for Suzuki, Grignard or silane coupling, as well as for Heck reactions. Thus, reaction of dibenzooxaphosphorin chloride with cyclohexylmagnesium chloride in THF/xylene gave 79% title phosphine, 2-(dicyclohexylphosphino)-2'-hydroxybiphenyl (II). PdCl2/II catalyzed the coupling of 4-MeC6H4MgCl with PhCl in THF to give 93% 4-MeC6H4Ph.

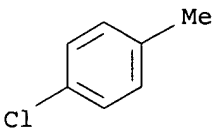
IC ICM C07F015-04
ICS C07F015-00; C07F009-50; B01J031-24; B01J031-06; C07B037-00; C07B049-00; C07B041-00; C07B043-00; C08F012-36; C08G083-00

CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 25, 78

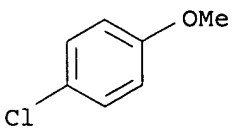
IT 80-10-4, Dichlorodiphenylsilane 100-42-5, reactions 100-59-4, Phenylmagnesium chloride **106-43-4**, 4-Chlorotoluene 108-90-7, Chlorobenzene, reactions 108-95-2, Phenol, reactions 109-09-1, 2-Chloropyridine 110-89-4, Piperidine, reactions 352-33-0, p-Fluorochlorobenzene **623-12-1**, p-Chloroanisole 696-61-7, 4-Tolylmagnesium chloride 934-56-5, Phenyltrimethylstannane **5980-97-2**, Mesitylboronic acid 9003-70-7, Styrene divinylbenzene resin 23708-48-7, Pentamethylenebismagnesium bromide 66107-32-2, 4-Cyanophenyl triflate 85676-85-3 304435-69-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of palladium and nickel complexes of biphenylylphosphines and application in catalytic carbon-carbon, carbon-nitrogen, and carbon-oxygen coupling reactions)

IT **106-43-4**, 4-Chlorotoluene **623-12-1**, p-Chloroanisole **5980-97-2**, Mesitylboronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of palladium and nickel complexes of biphenylylphosphines and application in catalytic carbon-carbon, carbon-nitrogen, and carbon-oxygen coupling reactions)

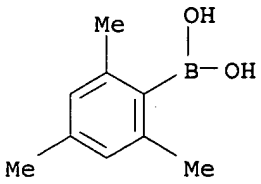
RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



RN 5980-97-2 HCAPLUS
CN Boronic acid, (2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



L36 ANSWER 13 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:765407 HCAPLUS
DOCUMENT NUMBER: 133:321695
TITLE: Preparation of biphenyls
INVENTOR(S): Yasuda, Toshiyuki; Hoshino, Manabu; Mori, Kunio
PATENT ASSIGNEE(S): Mitsubishi Rayon Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000302720	A2	20001031	JP 1999-116201	19990423

OTHER SOURCE(S): CASREACT 133:321695; MARPAT 133:321695

AB Title compds. I (R, A = H, C1-6 alkyl, Ph, C2-6 alkenyl, C2-6 alkynyl, C1-6 alkoxy, etc.; D = phenylene, naphthylene, pyridinediyl, quinolinediyl, pyrimidinediyl, etc.) are prepd. by reaction of arylboric acids II (R = same as I; Y = OH, C1-6 alkoxy, phenoxy, cyclohexyloxy, etc.) or III (R = same as I) with ADX (A, D = same as above; X = Cl, Br, I, mesylate group, arenesulfonate group) in the presence of bases, arom. hydrocarbon solvents, tertiary phosphines or phosphites, Ni salts, and alcs. P-methylphenylboric acid was reacted with p-ClC6H4CHO in the presence of PPh3, NiCl2, EtOH, and K3PO4.nH2O in PhMe at 80.degree. for 7 h to give 90% 4-formyl-4'-methyl-1,1-biphenyl.

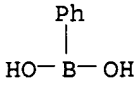
IC ICM C07C045-68
ICS B01J031-24; C07C041-30; C07C043-205; C07C047-546; C07C253-30; C07C255-50; C07D213-127; C07D213-16; C07B061-00

CC 25-2 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

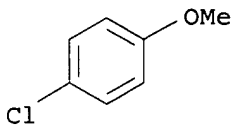
IT 64-17-5, Ethanol, reactions **98-80-6**, Phenylboric acid 104-88-1, p-Chlorobenzaldehyde, reactions 623-03-0, p-Chlorobenzonitrile **623-12-1**, 4-Chloroanisole 626-60-8, 3-Chloropyridine **5720-05-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biphenyls by condensation of arylboric acid with arom. compds.)

IT **98-80-6**, Phenylboric acid **623-12-1**, 4-Chloroanisole **5720-05-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biphenyls by condensation of arylboric acid with arom. compds.)

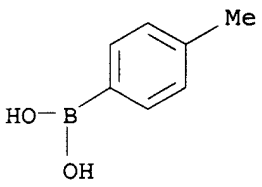
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



RN 5720-05-8 HCAPLUS
CN Boronic acid, (4-methylphenyl)- (9CI) (CA INDEX NAME)

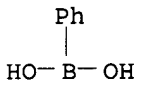


L36 ANSWER 14 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:765393 HCAPLUS
DOCUMENT NUMBER: 133:321694
TITLE: Preparation of biphenyls
INVENTOR(S): Miyaura, Sadao; Yasuda, Toshiyuki; Hoshino, Manabu; Mori, Kunio
PATENT ASSIGNEE(S): Mitsubishi Rayon Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

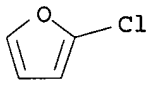
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000302697	A2	20001031	JP 1999-116200	19990423

OTHER SOURCE(S): CASREACT 133:321694; MARPAT 133:321694
AB Title compds. I (R, A = H, C1-6 alkyl, Ph, C2-6 alkenyl, C2-6 alkynyl, C1-6 alkoxy, etc.; D = phenylene, naphthylene, pyridinediyl, quinolinediyl; pyrimidinediyl, etc.) are prepd. by reaction of arylboric acids II (R = same as I; Y = OH, C1-6 alkoxy, phenoxy, cyclohexyloxy, etc.) with ADX (A, D = same as above; X = Cl, Br, I, mesylate group, arenesulfonate group) in the presence of divalent Ni, bases, arom. hydrocarbon solvents, and 0.5-10-fold (mol, based on I) of H2O or alcs. P-methylphenylboric acid was reacted with p-ClC6H4CHO in the presence of Cl2Ni(PPh3)2 and K3PO4.2H2O in PhMe at 80.degree. for 3 h to give 99% 4-formyl-4'-methyl-1,1-biphenyl.
IC ICM C07B037-04

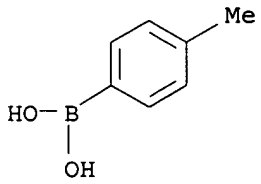
ICS B01J031-24; C07C045-68; C07C047-546; C07C253-30; C07C255-50; C07B061-00
CC 25-2 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 64-17-5, Ethanol, reactions 67-56-1, Methanol, reactions 80-00-2 96-43-5, 2-Chlorothiophene 97-50-7 **98-80-6**, Phenylboric acid 104-88-1, p-Chlorobenzaldehyde, reactions 106-47-8, p-Chloroaniline, reactions 610-96-8, Methyl o-chlorobenzoate 623-03-0, p-Chlorobenzonitrile 626-60-8, 3-Chloropyridine 698-69-1, p-Chloro-N,N-dimethylaniline 873-32-5, o-Chlorobenzonitrile 2845-89-8 2920-38-9, [1,1'-Biphenyl]-4-carbonitrile **3187-94-8**, 2-Chlorofuran **5720-05-8** 7732-18-5, Water, reactions 91105-99-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biphenyls by condensation of aryl borates with arom. compds. in presence of water or alcs.)
IT **98-80-6**, Phenylboric acid **3187-94-8**, 2-Chlorofuran **5720-05-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biphenyls by condensation of aryl borates with arom. compds. in presence of water or alcs.)
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



RN 3187-94-8 HCAPLUS
CN Furan, 2-chloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 5720-05-8 HCAPLUS
CN Boronic acid, (4-methylphenyl)- (9CI) (CA INDEX NAME)



L36 ANSWER 15 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:687982 HCAPLUS
DOCUMENT NUMBER: 133:252318
TITLE: Preparation of biaryls and arylamines via cross-coupling reactions of aryl halides with arylboronic acids or amines in presence of phosphine oxides and transition metals as catalysts
INVENTOR(S): Li, George Y.

PATENT ASSIGNEE(S): E. I. Du Pont De Nemours and Company, USA
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6124462	A	20000926	US 1999-451150	19991130
US 6291722	B1	20010918	US 2000-602714	20000626
WO 2001040147	A1	20010607	WO 2000-US18586	20000707
W: CA, JP				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1235764	A1	20020904	EP 2000-948591	20000707
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
US 2002137974	A1	20020926	US 2001-900353	20010706

PRIORITY APPLN. INFO.:
US 1999-451150 A2 19991130
US 2000-602714 A 20000626
WO 2000-US18586 W 20000707
US 2001-274530P P 20010309

OTHER SOURCE(S): CASREACT 133:252318; MARPAT 133:252318

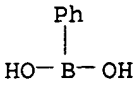
AB Phosphine oxide compds. were used with transition metals, preferably palladium, to produce biaryls and arylamines via cross-coupling reactions with aryl halides and arylboronic acids or amines. E.g., (Me3C)2P(O)H and Pd2(dba)3 catalyzed the reaction of PhCl and piperidine to give 51% N-phenylpiperidine. E.g., the same system catalyzed the reaction of PhCl and PhB(OH)2 to give 88% biphenyl.

IC ICM C07D211-00
NCL 546184000
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 25

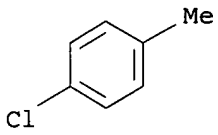
IT 62-53-3, Benzenamine, reactions 75-64-9, tert-Butylamine, reactions
98-56-6, 4-Chlorobenzotrifluoride **98-80-6**, Phenylboronic acid
100-58-3, Phenylmagnesium bromide **106-43-4**, 4-Chlorotoluene
106-49-0, p-Toluidine, reactions 108-90-7, Chlorobenzene, reactions
110-89-4, Piperidine, reactions 151-10-0, 1,3-Dimethoxybenzene
623-12-1, 4-Chloroanisole 644-97-3, Dichlorophenylphosphine
766-51-8, 2-Chloroanisole 1068-55-9, Isopropylmagnesium chloride
5720-05-8, 4-Methylphenylboronic acid **5720-07-0**,
4-Methoxyphenylboronic acid 7719-12-2, Trichlorophosphine 7789-60-8,
Tribromophosphine 13716-10-4, Chlorodi-tert-butylphosphine
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biaryls and arylamines via cross-coupling reactions of aryl halides with arylboronic acids or amines in presence of phosphine oxides and transition metals as catalysts)

IT **98-80-6**, Phenylboronic acid **106-43-4**, 4-Chlorotoluene
623-12-1, 4-Chloroanisole **5720-05-8**,
4-Methylphenylboronic acid **5720-07-0**, 4-Methoxyphenylboronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biaryls and arylamines via cross-coupling reactions of aryl halides with arylboronic acids or amines in presence of phosphine oxides and transition metals as catalysts)

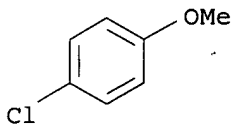
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



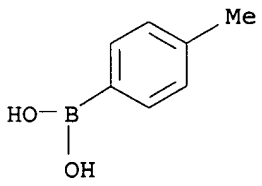
RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



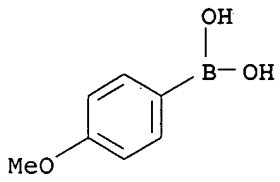
RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



RN 5720-05-8 HCAPLUS
CN Boronic acid, (4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 5720-07-0 HCAPLUS
CN Boronic acid, (4-methoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 16 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:261550 HCAPLUS
DOCUMENT NUMBER: 133:30370
TITLE: Biaryls via Suzuki cross-couplings catalyzed by nickel

on charcoal

AUTHOR(S): Lipshutz, Bruce H.; Sclafani, Joseph A.; Blomgren, Peter A.

CORPORATE SOURCE: Department of Chemistry & Biochemistry, University of California, Santa Barbara, CA, 93106-9510, USA

SOURCE: Tetrahedron (2000), 56(15), 2139-2144
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:30370

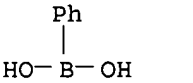
AB Using the heterogeneous catalyst Ni/C, biaryl bonds can be made between functionalized aryl chlorides and boronic acids in good isolated yields. A std. set of conditions was developed which applies to a variety of reaction partners. For example, the coupling reaction of 1-chloro-4-methoxybenzene with phenylboronic acid in the presence of nickel/charcoal and lithium bromide gave 4-methoxy-[1,1'-biphenyl]. Similarly, coupling of (4-methoxyphenyl)diphenylphosphine with phenylboronic acid also gave 4-methoxy-[1,1'-biphenyl] in good yield.

CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 25

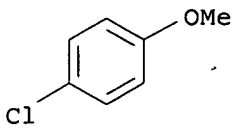
IT **98-80-6**, Phenylboronic acid 99-91-2 104-88-1, 4-Chlorobenzaldehyde, reactions 108-41-8, 1-Chloro-3-methylbenzene 134-85-0, 4-Chlorobenzophenone **623-12-1**, 1-Chloro-4-methoxybenzene 873-32-5, 2-Chlorobenzonitrile 896-89-9, (4-Methoxyphenyl)diphenylphosphine **1423-26-3**, [3-(Trifluoromethyl)phenyl]boronic acid **5720-05-8**, (4-Methylphenyl)boronic acid **5720-07-0**, (4-Methoxyphenyl)boronic acid 6165-69-1, (3-Thienyl)boronic acid 13922-41-3, (1-Naphthalenyl)boronic acid 39890-95-4, 2-Chloro-6-(trifluoromethyl)pyridine 85417-80-7, (3,4-Dimethoxyphenyl)diphenylphosphine 273937-68-1, 8-Chloro-5-methoxyquinoline
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biaryls via Suzuki cross-couplings catalyzed by nickel on charcoal)

IT **98-80-6**, Phenylboronic acid **623-12-1**, 1-Chloro-4-methoxybenzene **1423-26-3**, [3-(Trifluoromethyl)phenyl]boronic acid **5720-05-8**, (4-Methylphenyl)boronic acid **5720-07-0**, (4-Methoxyphenyl)boronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biaryls via Suzuki cross-couplings catalyzed by nickel on charcoal)

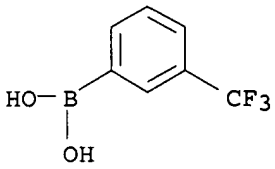
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



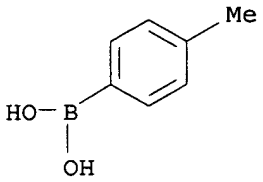
RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



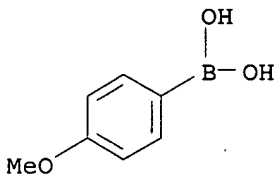
RN 1423-26-3 HCAPLUS
CN Boronic acid, [3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 5720-05-8 HCAPLUS
CN Boronic acid, (4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 5720-07-0 HCAPLUS
CN Boronic acid, (4-methoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 17 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:248593 HCAPLUS
DOCUMENT NUMBER: 133:43406
TITLE: Efficient Palladium-Catalyzed N-Arylation of Indoles
AUTHOR(S): Old, David W.; Harris, Michele C.; Buchwald, Stephen L.
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SOURCE: Organic Letters (2000), 2(10), 1403-1406
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:43406

AB The N-arylation of indoles, including a variety of substituted ones, has been carried out using bulky, electron-rich phosphines as the supporting ligand in combination with Pd2(dba)3. Using this catalyst system, the efficient coupling of indole and a variety of substituted indoles with aryl iodides, bromides, chlorides, and triflates can be achieved.

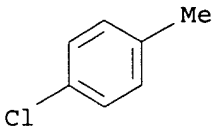
CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

IT 91-55-4, 2,3-Dimethylindole 95-20-5, 2-Methylindole 104-92-7, 4-Bromoanisole 106-38-7, 4-Bromotoluene **106-43-4**, 4-Chlorotoluene 109-04-6, 2-Bromopyridine 120-72-9, Indole, reactions 399-52-0, 5-Fluoroindole 460-00-4, 4-Bromofluorobenzene 553-94-6, Bromo-p-xylene 556-96-7, 5-Bromo-m-xylene 583-55-1, 2-Bromoiodobenzene 586-77-6, N,N-Dimethyl-4-bromoaniline 619-42-1, Methyl 4-bromobenzoate 624-31-7, 4-Iodotoluene 626-55-1, 3-Bromopyridine 778-82-5 782-17-2 948-65-2, 2-Phenylindole 1006-94-6, 5-Methoxyindole 1126-46-1, Methyl 4-chlorobenzoate 2142-63-4 2398-37-0, 3-Bromoanisole 3972-65-4, 4-Bromo-tert-butylbenzene 5798-75-4, Ethyl 4-bromobenzoate 7073-94-1, 2-Isopropylbromobenzene 13716-10-4, Di-tert-butylchlorophosphine 13922-41-3, 1-Naphthylboronic acid 15499-27-1 16523-54-9, Chlorodicyclohexylphosphine 17763-70-1 17789-14-9 22867-74-9, 7-Ethylindole 66107-29-7 207611-58-3 251320-89-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(palladium-catalyzed N-arylation of indoles)

IT 18937-92-3P **89787-12-2P**, 2-Isopropylphenylboronic acid
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(palladium-catalyzed N-arylation of indoles)

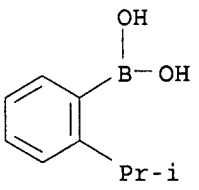
IT **106-43-4**, 4-Chlorotoluene
RL: RCT (Reactant); RACT (Reactant or reagent)
(palladium-catalyzed N-arylation of indoles)

RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



IT **89787-12-2P**, 2-Isopropylphenylboronic acid
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(palladium-catalyzed N-arylation of indoles)

RN 89787-12-2 HCAPLUS
CN Boronic acid, [2-(1-methylethyl)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 18 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:246770 HCAPLUS
DOCUMENT NUMBER: 133:30542
TITLE: Versatile Catalysts for the Suzuki Cross-Coupling of Arylboronic Acids with Aryl and Vinyl Halides and Triflates under Mild Conditions
AUTHOR(S): Littke, Adam F.; Dai, Chaoyang; Fu, Gregory C.
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SOURCE: Journal of the American Chemical Society (2000), 122(17), 4020-4028
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:30542

AB Through the use of Pd2(dba)3/P(t-Bu)3 as a catalyst, a wide range of aryl and vinyl chlorides, bromides, and iodides undergo Suzuki cross-coupling with arylboronic acids in very good yield, typically at room temp. In the presence of Pd(OAc)2 and PCy3, a diverse array of aryl and vinyl triflates react cleanly at room temp. with arylboronic acids. The catalyst systems Pd2(dba)3/(Me3C)3P and Pd(OAc)2/PCy3 cover a broad spectrum of commonly encountered substrates for Suzuki couplings. Selective cross-coupling of an aryl chloride in the presence of an aryl triflate was performed in the presence of Pd2(dba)3/P(t-Bu)3 while selective coupling of an aryl triflate in the presence of an aryl chloride was performed in the presence of Pd(OAc)2/PCy3. Both Suzuki cross-coupling catalyst systems are effective at low loadings [as low as 0.005 mol% Pd2(dba)3/0.01 mol% P(Bu-t)3], even with aryl chloride substrates [0.05 - 3 mol% Pd2(dba)3/0.12 - 6 mol% P(Bu-t)3]. Preliminary mechanistic work indicates that a palladium monophosphine complex is the active catalyst in the cross-coupling of aryl halides.

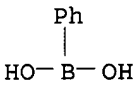
CC 25-1 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT 95-46-5, 2-Bromotoluene 95-49-8, 2-Chlorotoluene **98-80-6**, Phenylboronic acid 99-90-1 99-91-2 104-92-7, 1-Bromo-4-methoxybenzene 106-39-8, 1-Bromo-4-chlorobenzene 106-41-2, 4-Bromophenol **106-43-4**, 4-Chlorotoluene 106-47-8, 4-Chloroaniline, reactions 108-90-7, Chlorobenzene, reactions 109-09-1, 2-Chloropyridine 513-37-1, 1-Chloro-2-methyl-1-propene 540-37-4, 4-Iodoaniline 576-22-7 586-77-6, 4-Bromo-N,N-dimethylaniline 615-37-2, 1-Iodo-2-methylbenzene **623-12-1**, 1-Chloro-4-methoxybenzene 626-60-8, 3-Chloropyridine 637-87-6, 1-Chloro-4-iodobenzene 696-62-8, 1-Iodo-4-methoxybenzene 873-32-5, 2-Chlorobenzonitrile 930-29-0 3017-70-7 3972-65-4, 1-Bromo-4-(tert-butyl)benzene **5720-05-8**, 4-Methylphenylboronic acid **5720-07-0**, 4-Methoxyphenylboronic acid **5980-97-2**, Mesitylboronic acid 6165-68-0, 2-Thienylboronic acid 6310-09-4, 5-Chloro-2-acetylthiophene 6781-98-2 6832-09-3 13329-40-3, 4-Iodoacetophenone **16419-60-6**, o-Tolylboronic acid 23525-05-5 29540-83-8 29540-84-9 35779-04-5 63076-51-7 66107-29-7 66107-30-0 66107-34-4 77412-96-5 96133-27-6 109613-00-5 **149104-90-5**, 4-Acetylphenylboronic acid 154318-75-9 229031-52-1 274257-34-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biphenyl and alkenylphenyl derivs. by selective Suzuki cross-coupling of aryl and alkenyl halides and triflates with arylboronic acids in the presence of palladium catalysts)

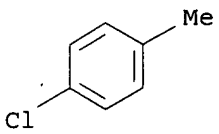
IT **98-80-6**, Phenylboronic acid **106-43-4**, 4-Chlorotoluene

623-12-1, 1-Chloro-4-methoxybenzene **5720-05-8**, 4-Methylphenylboronic acid **5720-07-0**, 4-Methoxyphenylboronic acid **5980-97-2**, Mesitylboronic acid **16419-60-6**, o-Tolylboronic acid **149104-90-5**, 4-Acetylphenylboronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biphenyl and alkenylphenyl derivs. by selective Suzuki cross-coupling of aryl and alkenyl halides and triflates with arylboronic acids in the presence of palladium catalysts)

RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



RN 623-12-1 HCAPLUS
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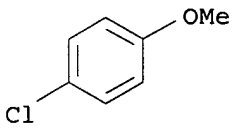

RN 5720-05-8 HCAPLUS
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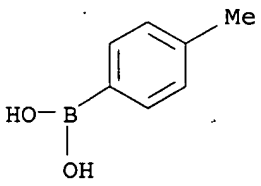
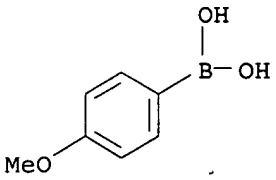
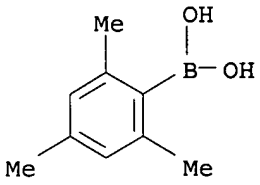


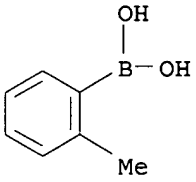
RN 5720-07-0 HCAPLUS
CN Boronic acid, (4-methoxyphenyl)- (9CI) (CA INDEX NAME)



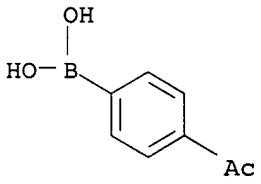
RN 5980-97-2 HCAPLUS
CN Boronic acid, (2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



RN 16419-60-6 HCAPLUS
CN Boronic acid, (2-methylphenyl)- (9CI) (CA INDEX NAME)



RN 149104-90-5 HCAPLUS
CN Boronic acid, (4-acetylphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 128 THERE ARE 128 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 19 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:53646 HCAPLUS
DOCUMENT NUMBER: 132:108101
TITLE: Biaryl phosphine and amine ligands for improved transition metal-catalyzed processes
INVENTOR(S): Buchwald, Stephen; Old, David W.; Wolfe, John P.; Palucki, Michael; Kamikawa, Ken; Chieffi, Andrew; Sadighi, Joseph P.; Singer, Robert A.; Ahman, Jens

PATENT ASSIGNEE(S): Massachusetts Institute of Technology, USA
SOURCE: PCT Int. Appl., 397 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000002887	A2	20000120	WO 1999-US15450	19990709
WO 2000002887	A3	20000629		
W: CA, JP				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6395916	B1	20020528	US 1998-113478	19980710
US 6307087	B1	20011023	US 1999-231315	19990113
CA 2336691	AA	20000120	CA 1999-2336691	19990709
EP 1097158	A2	20010509	EP 1999-933785	19990709
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002520328	T2	20020709	JP 2000-559117	19990709

PRIORITY APPLN. INFO.:
US 1998-113478 A 19980710
US 1998-196855 A 19981120
US 1999-231315 A 19990113
US 1999-239024 A 19990127
WO 1999-US15450 W 19990709

OTHER SOURCE(S): MARPAT 132:108101

AB The present invention relates to the prepn. of novel biaryl phosphine and amine ligands (I) [wherein A and B = independently fused monocyclic or polycyclic cycloalkyl, cycloalkenyl, aryl, or heterocyclic rings of 4-8 atoms; X = NR2, PR2, AsR2, OR, or SR; Y = NR2, PR2, AsR2, OR, SR, SiR3, alkyl, or H; R-R6 = independently H, halogen, (hetero)alkyl, alkenyl, alkynyl, hydroxy, alkoxy, silyloxy, amino, nitro, sulfhydryl, amide, carbonyl, ketone, anhydride, silyl, thioalkyl, ketone, ester, nitrile, (hetero)aryl, etc.] for transition metals and their use in metal-catalyzed carbon-heteroatom and carbon-carbon bond-forming reactions. Unexpected improvements over the prior art were demonstrated in transition metal-catalyzed aryl amination reactions, Suzuki couplings giving both biaryl and alkylaryl products, arylations and vinylations at the position .alpha. to carbonyl groups, and carbon-oxygen bond formation. The ligands and methods of the invention enable transformations utilizing aryl chlorides and bromides at room temp. at synthetically useful rates with extremely small amts. of catalyst relative to the limiting reagent. For example, coupling of p-chlorobenzonitrile and morpholine was catalyzed by 2.5 mol% Pd2(dba)3, 7.5 mol% of 2-(N,N-dimethylamino)-2'-(dicyclohexylphosphino)biphenyl, and NaOBu-t in DME at room temp. to provide 4-(4-morpholinyl)benzonitrile in 96% yield. Thus, the subject processes provide improvements in many features of the transition metal-catalyzed reactions, including the range of suitable substrates, reaction conditions, and efficiency.

IC ICM C07F009-02
CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 25
IT 698-00-0P **4688-76-0P** 18937-92-3P 20837-12-1P, 2-Bromo-2'-methoxy-1,1'-biphenyl 59734-92-8P 75295-57-7P **89291-23-6P** **89787-12-2P**, 2-Isopropylphenylboronic acid **128796-39-4P**, 4-(Trifluoromethyl)phenylboronic acid 224311-57-3P 224311-58-4P 224311-59-5P 251320-87-3P, 2-Bromo-2'-methylbiphenyl 251320-89-5P, 2-Bromo-2'-isopropylbiphenyl 255837-15-1P,

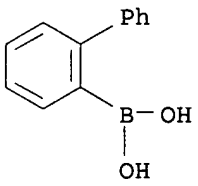
2-Bromo-4'-(trifluoromethyl)biphenyl 255837-16-2P 255837-18-4P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; **prepn**. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT 62-53-3, Benzenamine, reactions 75-97-8 88-05-1 88-69-7 90-04-0 91-55-4 93-55-0, Propiophenone 95-65-8 95-68-1 95-72-7 96-22-0, 3-Pentanone 98-54-4 **98-80-6** 98-86-2, reactions 99-02-5 99-90-1 99-91-2 100-00-5, 1-Chloro-4-nitrobenzene 100-01-6, reactions 100-42-5, reactions 100-46-9, Benzenemethanamine, reactions 100-61-8, reactions 103-69-5 103-88-8, 4'-Bromoacetanilide 104-92-7 104-94-9 105-53-3, Diethyl malonate 106-38-7 106-39-8 106-41-2, 4-Bromophenol **106-43-4** 106-49-0, reactions 108-41-8 108-44-1, reactions 108-91-8, Cyclohexanamine, reactions 108-94-1, Cyclohexanone, reactions 109-01-3 109-04-6 109-09-1 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-26-2, 1-Hexanamine 111-92-2 119-61-9, Benzophenone, reactions 120-72-9, Indole, reactions 122-00-9 122-39-4, Diphenylamine, reactions 123-75-1, Pyrrolidine, reactions 141-97-9 280-64-8, 9-BBN 392-83-6, 2-Bromobenzotrifluoride 399-52-0 402-43-7, 4-(Trifluoromethyl)phenyl bromide 460-00-4, 1-Bromo-4-fluorobenzene 502-42-1, Cycloheptanone 504-02-9, 1,3-Cyclohexanedione 529-34-0 530-93-8, .beta.-Tetralone 540-88-5, tert-Butyl acetate 553-94-6 556-96-7 557-93-7, 2-Bromopropene 563-80-4 565-69-5 565-80-0 576-22-7 576-26-1 583-53-9, 1,2-Dibromobenzene 583-55-1, 2-Bromoiodobenzene 586-77-6 588-72-7, trans-.beta.-Bromostyrene 590-15-8, trans-1-Bromopropene 591-20-8 592-41-6, 1-Hexene, reactions 615-36-1, 2-Bromoaniline 618-45-1 618-89-3 619-42-1 623-00-7, 4-Bromobenzonitrile 623-03-0 **623-12-1** 624-31-7 626-55-1, 3-Bromopyridine 626-60-8, 3-Chloropyridine 645-36-3 765-30-0, Cyclopropylamine 766-51-8 766-84-7 778-82-5 782-17-2 872-31-1, 3-Bromothiophene 873-32-5, 2-Chlorobenzonitrile 930-29-0, 1-Chlorocyclopentene 931-51-1, Cyclohexylmagnesium chloride 948-65-2 1003-09-4, 2-Bromothiophene 1013-88-3, Benzophenone imine 1079-66-9, Chlorodiphenylphosphine 1122-91-4, 4-Bromobenzaldehyde 1122-95-8 1126-46-1 1450-65-3 1590-08-5 2038-03-1, 4-Morpholineethanamine 2052-07-5, 2-Bromobiphenyl 2142-68-9, 2'-Chloroacetophenone 2398-37-0 2635-13-4 2845-89-8 2856-63-5, 2-Chlorobenzyl cyanide 2905-65-9 3972-65-4, 1-Bromo-4-t-butylbenzene 4079-52-1 4541-32-6 5350-57-2 5619-07-8, DL-Phenylalanine methyl ester hydrochloride **5720-06-9** 5798-75-4, Ethyl 4-bromobenzoate 5892-99-9 6781-98-2 7051-16-3 7073-94-1, 2-Bromoisopropylbenzene 7524-50-7, L-Phenylalanine methyl ester hydrochloride 7598-28-9 13716-10-4, Chlorodi-tert-butylphosphine 13922-41-3, 1-Naphthylboronic acid 15499-27-1 16081-16-6 **16419-60-6** 16523-54-9, Chlorodicyclohexylphosphine 17496-14-9, 2-Methylindanone 17763-70-1 17763-80-3 17789-14-9, 2-(3-Bromophenyl)1,3-dioxolane **17933-03-8** 18982-54-2, 2-Bromobenzyl alcohol **22237-13-4**, 4-Ethoxyphenylboronic acid 22867-74-9 24544-04-5 27505-78-8 27752-24-5 36800-95-0, 4-Cyanophenyl tosylate **40138-16-7**, 2-Formylphenylboronic acid 41085-43-2, 2-Bromo-3-nitrotoluene 41492-05-1 42371-64-2 53847-33-9 66107-29-7 66107-32-2 74866-28-7, 2,2'-Dibromo-1,1'-binaphthyl **100379-00-8** 100717-47-3 109613-00-5 112042-84-9 154318-75-9 157282-19-4 158266-43-4 **204841-19-0**, 3-Acetylphenylboronic acid 207611-58-3 255837-20-8 255837-21-9 255837-22-0 255837-23-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; **prepn**. of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki

couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

IT **4688-76-0P 89291-23-6P 89787-12-2P,** 2-Isopropylphenylboronic acid **128796-39-4P,** 4-(Trifluoromethyl)phenylboronic acid
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; **prepn.** of biaryl phosphine and amine ligands for improved palladium-catalyzed amination reactions, Suzuki couplings, arylations, vinylations, and carbon-oxygen bond formation reactions)

RN 4688-76-0 HCAPLUS
CN Boronic acid, [1,1'-biphenyl]-2-yl- (9CI) (CA INDEX NAME)



RN 89291-23-6 HCAPLUS
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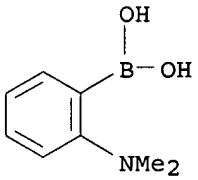

RN 89787-12-2 HCAPLUS
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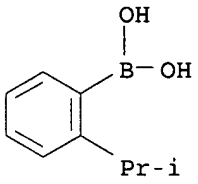

RN 128796-39-4 HCAPLUS
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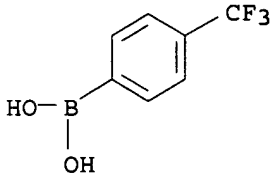
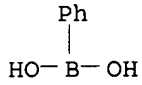


IT **98-80-6 106-43-4 623-12-1 5720-06-9**
16419-60-6 17933-03-8 22237-13-4,
4-Ethoxyphenylboronic acid **40138-16-7**, 2-Formylphenylboronic
acid **100379-00-8 204841-19-0**, 3-Acetylphenylboronic
acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; **prepn**. of biaryl phosphine and amine
ligands for improved palladium-catalyzed amination reactions, Suzuki
couplings, arylations, vinylations, and carbon-oxygen bond formation
reactions)

RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



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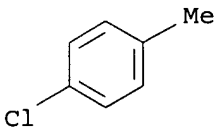
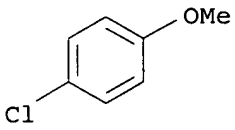
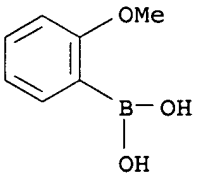
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



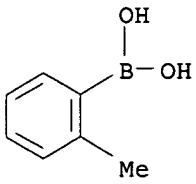
RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



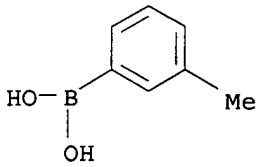
RN 5720-06-9 HCAPLUS
CN Boronic acid, (2-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 16419-60-6 HCAPLUS
CN Boronic acid, (2-methylphenyl)- (9CI) (CA INDEX NAME)



RN 17933-03-8 HCAPLUS
CN Boronic acid, (3-methylphenyl)- (9CI) (CA INDEX NAME)



RN 22237-13-4 HCAPLUS
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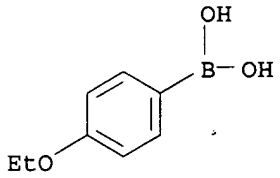
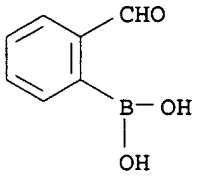
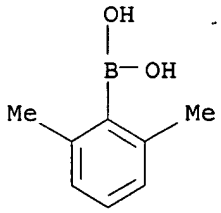


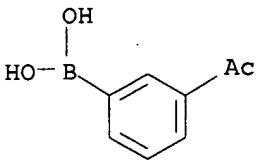
RN 40138-16-7 HCAPLUS
CN Boronic acid, (2-formylphenyl)- (9CI) (CA INDEX NAME)



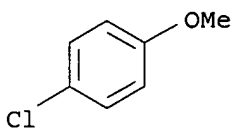
RN 100379-00-8 HCAPLUS
CN Boronic acid, (2,6-dimethylphenyl)- (9CI) (CA INDEX NAME)



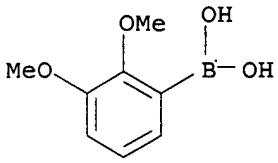
RN 204841-19-0 HCAPLUS
CN Boronic acid, (3-acetylphenyl)- (9CI) (CA INDEX NAME)



L36 ANSWER 20 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:712076 HCAPLUS
DOCUMENT NUMBER: 132:122339
TITLE: Directed ortho-metalation and Suzuki-Miyaura cross-coupling connections: regiospecific synthesis of all isomeric chlorodihydroxybiphenyls for microbial degradation studies of PCBs
AUTHOR(S): Nerdinger, S.; Marchhart, R.; Riebel, P.; Kendall, C.; Johnson, M. R.; Yin, C.-F.; Snieckus, V.; Eltis, L. D.
CORPORATE SOURCE: Guelph-Waterloo Centre for Graduate Work in Chemistry, University of Waterloo, Waterloo, ON, N2L 3G1, Can.
SOURCE: Chemical Communications (Cambridge) (1999), (22), 2259-2260
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 2,3-(HO)2C6H3C6H4R [R = H, 2-Cl, 3-Cl, 4-Cl] and 3,1,2-Ph(HO)2C6H2R [R = 4-Cl, 5-Cl, 6-Cl] have been regioselectively synthesized in good overall yields by a combination of directed ortho metalation and Suzuki-Miyaura cross-coupling.
CC 25-10 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 91-16-7, 1,2-Dimethoxybenzene 108-86-1, Bromobenzene, reactions
615-41-8, 1-Chloro-2-iodobenzene **623-12-1**, 4-Chloroanisole
625-99-0, 1-Chloro-3-iodobenzene 637-87-6, 1-Chloro-4-iodobenzene
826-26-6 115377-97-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(regiospecific prepn. of all isomeric chlorodihydroxybiphenyls)
IT **40972-86-9P** 256431-54-6P 256431-55-7P 256431-57-9P
256431-59-1P 256431-60-4P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(regiospecific **prepn.** of all isomeric chlorodihydroxybiphenyls)
IT **623-12-1**, 4-Chloroanisole
RL: RCT (Reactant); RACT (Reactant or reagent)
(regiospecific prepn. of all isomeric chlorodihydroxybiphenyls)
RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



IT **40972-86-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(regiospecific **prepn.** of all isomeric chlorodihydroxybiphenyls)
RN 40972-86-9 HCAPLUS
CN Boronic acid, (2,3-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

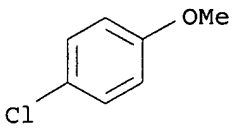
L36 ANSWER 21 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:261305 HCAPLUS
DOCUMENT NUMBER: 130:337883
TITLE: Novel electron-rich bulky phosphine ligands facilitate the palladium-catalyzed preparation of diaryl ethers
AUTHOR(S): Aranyos, Attila; Old, David W.; Kiyomori, Ayumu; Wolfe, John P.; Sadighi, Joseph P.; Buchwald, Stephen L.
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SOURCE: Journal of the American Chemical Society (1999), 121(18), 4369-4378
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:337883
AB A general method for the palladium-catalyzed formation of diaryl ethers, e.g., PhOC6H4COMe-4, is described. Electron-rich, bulky aryldialkylphosphine ligands, e.g., 2-PhC6H4P(CMe3)2, in which the two alkyl groups are either tert-Bu or 1-adamantyl, are the key to the success of the transformation. A wide range of electron-deficient, electronically neutral and electron-rich aryl bromides, chlorides, and triflates can be combined with a variety of phenols with the use of sodium hydride or potassium phosphate as base in toluene at 100.degree.C. The bulky yet basic nature of the phosphine ligand is thought to be responsible for increasing the rate of reductive elimination of the diaryl ether from palladium.
CC 25-9 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 88-69-7, 2-Isopropylphenol 95-48-7, reactions 95-65-8 95-72-7 98-54-4, 4-tert-Butylphenol 99-90-1 104-92-7, 4-Bromomethoxybenzene 106-39-8, 4-Bromochlorobenzene 106-44-5, reactions 108-95-2, Phenol, reactions 150-76-5, 4-Methoxyphenol 553-94-6 556-96-7 576-26-1 583-55-1, 2-Bromoiodobenzene 618-45-1, 3-Isopropylphenol 619-42-1, Methyl 4-bromobenzoate 623-03-0, 4-Chlorobenzonitrile **623-12-1** 768-90-1, 1-Bromoadamantane 1013-88-3 2052-07-5, 2-Bromobiphenyl 2142-63-4, 3-Bromoacetophenone 2398-37-0 3972-65-4, 4-tert-Butylbromobenzene 5892-99-9 13716-10-4 15499-27-1 16081-16-6 41492-05-1 74866-28-7 109613-00-5 154318-75-9

213697-67-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of diaryl ethers using palladium catalyst and phosphine ligands)

IT **4688-76-0P** 75295-57-7P 224311-57-3P 224311-58-4P
224311-59-5P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(**prepn.** of diaryl ethers using palladium catalyst and phosphine ligands)

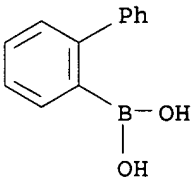
IT **623-12-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of diaryl ethers using palladium catalyst and phosphine ligands)

RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



IT **4688-76-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(**prepn.** of diaryl ethers using palladium catalyst and phosphine ligands)

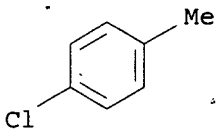
RN 4688-76-0 HCAPLUS
CN Boronic acid, [1,1'-biphenyl]-2-yl- (9CI) (CA INDEX NAME)



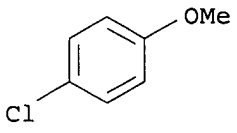
REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 22 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:577201 HCAPLUS
DOCUMENT NUMBER: 129:275663
TITLE: A Highly Active Catalyst for Palladium-Catalyzed Cross-Coupling Reactions: Room-Temperature Suzuki Couplings and Amination of Unactivated Aryl Chlorides
AUTHOR(S): Old, David W.; Wolfe, John P.; Buchwald, Stephen L.
CORPORATE SOURCE: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SOURCE: Journal of the American Chemical Society (1998), 120(37), 9722-9723
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

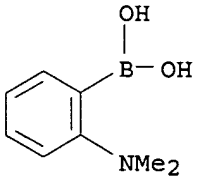
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:275663
AB Pd2(dba)3 and ligand 2-(dicyclohexylphosphino)-2'-(dimethylamino)biphenyl catalyzed the amination of aryl chloride or bromides at room temp. Also, Pd2(dba)3 or Pd(OAc)2 and ligand 2-(dicyclohexylphosphino)-2'-(dimethylamino)biphenyl catalyzed the Suzuki coupling of aryl chloride or bromides with boron reagents at room temp.
CC 25-1 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT 95-72-7 98-80-6 99-90-1 99-91-2 100-46-9, Benzylamine, reactions 100-61-8, reactions 106-38-7 **106-43-4** 106-49-0, p-Toluidine, reactions 110-91-8, Morpholine, reactions 111-26-2, Hexylamine 111-92-2, Dibutylamine 553-94-6 556-96-7 563-80-4 565-69-5 576-22-7 583-55-1, 2-Bromoiodobenzene 619-42-1 623-03-0 **623-12-1** 698-00-0 1126-46-1 5720-06-9 16523-54-9, Chlorodicyclohexylphosphine 17933-03-8 42371-64-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(palladium-catalyzed Suzuki coupling reactions or amination of aryl chlorides or aryl bromides)
IT **89291-23-6P** 213697-67-7P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(palladium-catalyzed Suzuki coupling reactions or amination of aryl chlorides or aryl bromides)
IT **106-43-4 623-12-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(palladium-catalyzed Suzuki coupling reactions or amination of aryl chlorides or aryl bromides)
RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



IT **89291-23-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(palladium-catalyzed Suzuki coupling reactions or amination of aryl chlorides or aryl bromides)
RN 89291-23-6 HCAPLUS
CN Boronic acid, [2-(dimethylamino)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 23 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:720354 HCAPLUS
DOCUMENT NUMBER: 127:330925
TITLE: Synthesis of Biaryls via a Nickel(0)-Catalyzed Cross-Coupling Reaction of Chloroarenes with Arylboronic Acids
AUTHOR(S): Saito, Syun; Oh-tani, Saori; Miyaura, Norio
CORPORATE SOURCE: Division of Molecular Chemistry Graduate School of Engineering, Hokkaido University, Sapporo, 060, USA
SOURCE: Journal of Organic Chemistry (1997), 62(23), 8024-8030
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 127:330925

AB The cross-coupling reaction of arylboronic acid with chloroarenes to give biaryls was carried out in high yields at 70-80 .degree.C in the presence of a nickel(0) catalyst and K3PO4 (3 equiv) in dioxane or benzene. The nickel(0) catalyst in situ prepd. from NiCl2.cntdot.L (L = dppf, 2PPh3) (3-10 mol %) and 4 equiv of BuLi at room temp. was recognized to be most effective. The reaction can be applicable to a wide range of chloroarenes having an electron-withdrawing or an electron-donating group such as 4-NC, 4-CHO, 2- or 4-CO2Me, 4-COMe, 4-NHAc, 4-Me, 4-OMe, 4-NH2, and 4-NMe2. The Hammett's plot of the substituent effect of chloroarenes revealed that the reaction involves a rate-detg. oxidative addn. of chloroarenes to the nickel(0) complex.

CC 21-2 (General Organic Chemistry)

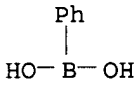
IT **98-80-6**, Phenylboronic acid 99-91-2 **106-43-4**, 4-Chlorotoluene 108-90-7, reactions 352-33-0, p-Chlorofluorobenzene 623-03-0 **623-12-1 1765-93-1** 2905-65-9 **5720-05-8 5720-07-0 149104-90-5**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(**prepn**. of biaryls via a nickel-catalyzed cross-coupling reaction of chloroarenes with arylboronic acids)

IT 97-50-7 100-00-5 104-88-1, reactions 106-47-8, reactions 108-41-8, 3-Chlorotoluene 539-03-7 610-96-8 612-62-4, 2-Chloroquinoline 698-69-1 1126-46-1 2845-89-8 3140-73-6 **5980-97-2** **16419-60-6** 17249-80-8, 3-Chlorothiophene 19219-99-9 25235-85-2 28045-90-1
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(**prepn**. of biaryls via a nickel-catalyzed cross-coupling reaction of chloroarenes with arylboronic acids)

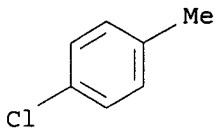
IT **98-80-6**, Phenylboronic acid **106-43-4**, 4-Chlorotoluene **623-12-1 1765-93-1 5720-05-8 5720-07-0 149104-90-5**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(**prepn.** of biaryls via a nickel-catalyzed cross-coupling reaction of chloroarenes with arylboronic acids)

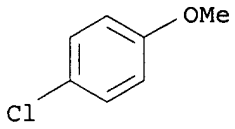
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



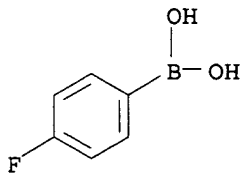
RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



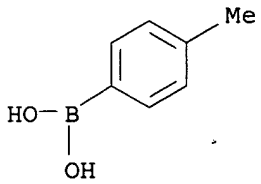
RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



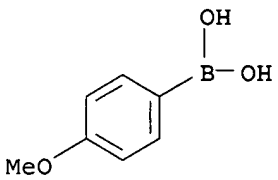
RN 1765-93-1 HCAPLUS
CN Boronic acid, (4-fluorophenyl)- (9CI) (CA INDEX NAME)



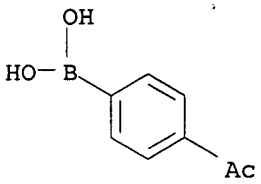
RN 5720-05-8 HCAPLUS
CN Boronic acid, (4-methylphenyl)- (9CI) (CA INDEX NAME)



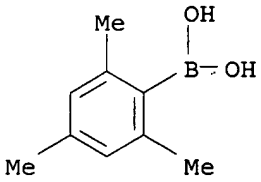
RN 5720-07-0 HCAPLUS
CN Boronic acid, (4-methoxyphenyl)- (9CI) (CA INDEX NAME)



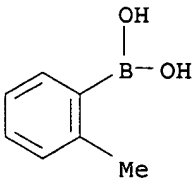
RN 149104-90-5 HCAPLUS
CN Boronic acid, (4-acetylphenyl)- (9CI) (CA INDEX NAME)



IT **5980-97-2 16419-60-6**
RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(**prepn**. of biaryls via a nickel-catalyzed cross-coupling reaction of chloroarenes with arylboronic acids)
RN 5980-97-2 HCAPLUS
CN Boronic acid, (2,4,6-trimethylphenyl)- (9CI) (CA INDEX NAME)



RN 16419-60-6 HCAPLUS
CN Boronic acid, (2-methylphenyl)- (9CI) (CA INDEX NAME)



L36 ANSWER 24 OF 26 HCAPLUS. COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:349325 HCAPLUS
DOCUMENT NUMBER: 127:81199

TITLE: Suzuki-type coupling of chloroarenes with arylboronic acids catalyzed by nickel complexes
AUTHOR(S): Indolese, Adriano F.
CORPORATE SOURCE: Catalysis Research, Novartis Services AG, Basel, CH-4002, Switz.
SOURCE: Tetrahedron Letters (1997), 38(20), 3513-3516
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

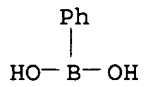
AB A Suzuki-type cross-coupling reaction of aryl chlorides with arylboronic acids using nickel-catalysts was described. The best results were obtained at 95 .degree.C in the presence of K3PO4 and in dioxane using Ni(dppf)Cl2. Unsym. biaryls with both electron-withdrawing and electron-donating functional groups were obtained in high yields.

CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

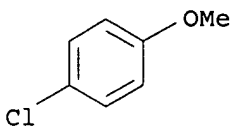
IT 90-13-1, 1-Chloronaphthalene 95-50-1, 1,2-Dichlorobenzene 98-56-6, 1-Chloro-4-(trifluoromethyl)benzene **98-80-6**, Phenylboronic acid 99-91-2 108-42-9, 3-Chloroaniline 587-04-2, 3-Chlorobenzaldehyde **623-12-1**, 4-Chloroanisole 873-32-5, 2-Chlorobenzonitrile 2367-91-1, 1-Chloro-2,5-difluorobenzene **5720-05-8**, 4-Methylphenylboronic acid 6165-68-0, 2-Thienylboronic acid **13331-27-6**, 3-Nitrophenylboronic acid **16419-60-6**, 2-Methylphenylboronic acid 179104-32-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biaryls via nickel-catalyzed Suzuki coupling of chloroarenes with arylboronic acids)

IT **98-80-6**, Phenylboronic acid **623-12-1**, 4-Chloroanisole **5720-05-8**, 4-Methylphenylboronic acid **13331-27-6**, 3-Nitrophenylboronic acid **16419-60-6**, 2-Methylphenylboronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biaryls via nickel-catalyzed Suzuki coupling of chloroarenes with arylboronic acids)

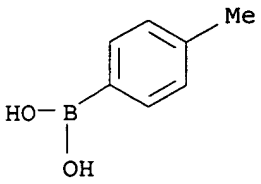
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



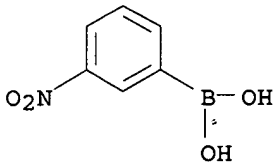
RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



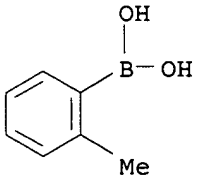
RN 5720-05-8 HCAPLUS
CN Boronic acid, (4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 13331-27-6 HCAPLUS
CN Boronic acid, (3-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 16419-60-6 HCAPLUS
CN Boronic acid, (2-methylphenyl)- (9CI) (CA INDEX NAME)

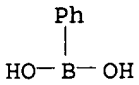


L36 ANSWER 25 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:271985 HCAPLUS
DOCUMENT NUMBER: 125:33269
TITLE: A synthesis of biaryls via nickel(0)-catalyzed cross-coupling reaction of chloroarenes with phenylboronic acids
AUTHOR(S): Saito, Syun; Sakai, Masaaki; Miyaura, Norio
CORPORATE SOURCE: Fac. Eng., Hokkaido Univ., Sapporo, 060, Japan
SOURCE: Tetrahedron Letters (1996), 37(17), 2993-6
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The cross-coupling reaction of phenylboronic acid with chloroarenes, e.g., 4-chlorobenzonitrile, to give biaryls, e.g., 4-phenylbenzonitrile, was carried out in high yields at 80.degree.C in the presence of nickel(0) catalyst and K3PO4 (3 equivs) in dioxane. The nickel(0) catalyst prepd. in situ from NiCl2(dppf) (10 mol%; dppf = 1,1'-bis(diphenylphosphino)ferrocene) and four equivs. of BuLi was the most effective. The reaction can be applicable for a wide range of chloroarenes having an electron-withdrawing or an electron-donating group such as 4-cyano-, 4-CHO, 2- or 4-CO2Me, 4-COMe, 4-NHAc, 3- or 4-Me, and 3- or 4-OMe, and 4-NH2.
CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

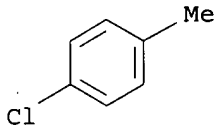
IT **98-80-6**, Phenylboronic acid 99-91-2 104-88-1, 4-Chlorobenzaldehyde, reactions **106-43-4**, 4-Chlorotoluene 106-47-8, 4-Chloroaniline, reactions 108-41-8, 3-Chlorotoluene 539-03-7, 4'-Chloroacetanilide 610-96-8, Methyl 2-chlorobenzoate 623-03-0, 4-Chlorobenzonitrile **623-12-1** 1126-46-1, Methyl 4-chlorobenzoate 2845-89-8, 3-Chloromethoxybenzene
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biaryls by nickel-catalyzed cross-coupling of chloroarenes with phenylboronic acid)

IT **98-80-6**, Phenylboronic acid **106-43-4**, 4-Chlorotoluene **623-12-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(**prepn**. of biaryls by nickel-catalyzed cross-coupling of chloroarenes with phenylboronic acid)

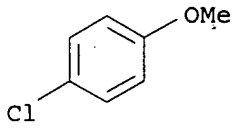
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)



L36 ANSWER 26 OF 26 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:406059 HCAPLUS
DOCUMENT NUMBER: 87:6059
TITLE: Reactions of diborane with organic derivatives of lithium, sodium, potassium and calcium
AUTHOR(S): Thorpe, F. G.; Pickles, G. M.; Podesta, J. C.
CORPORATE SOURCE: Dep. Chem., Univ. Lancaster, Lancaster, Engl.
SOURCE: J. Organomet. Chem. (1977), 128(3), 305-12
CODEN: JORCAI
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The reactions of org. halides (e.g., PhBr) with diborane in THF in the presence of Li, Na, K, Ca were examd. Phenols (or alcs.) are obtained in good yields by H2O2 oxidn. of the products of the above reactions,

indicating the formation of organoboron intermediates by a transmetalation process. Arylboronic acids can also be obtained in good yield by the hydrolysis of the products of the reactions involving Li. These one-step reactions are superior to analogous two-step reactions in which pre-formed organolithium reagents react with diborane.

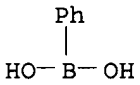
CC 29-4 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 24, 25, 26

IT **98-80-6P 5720-07-0P 17933-03-8P**
63139-21-9P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)

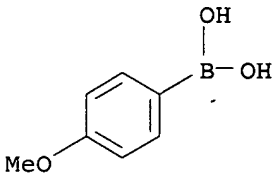
IT 95-46-5 100-39-0 104-92-7 106-38-7 **106-43-4** 106-94-5
108-41-8 108-85-0 108-86-1, reactions 108-90-7, reactions 109-65-9
110-53-2 111-25-1 111-83-1 112-29-8 112-82-3 137-43-9 507-19-7
542-18-7 544-77-4 576-83-0 588-96-5 591-17-3 591-50-4
623-12-1 624-31-7 625-95-6 696-62-8 1585-07-5 1973-22-4
2398-37-0 23074-36-4
RL: RCT (Reactant)
(reaction of, with diborane in presence of alk. metals)

IT **98-80-6P 5720-07-0P 17933-03-8P**
63139-21-9P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)

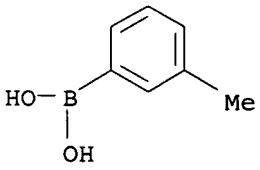
RN 98-80-6 HCAPLUS
CN Boronic acid, phenyl- (9CI) (CA INDEX NAME)



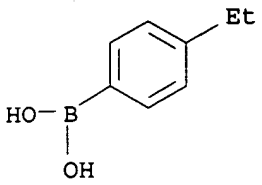
RN 5720-07-0 HCAPLUS
CN Boronic acid, (4-methoxyphenyl)- (9CI) (CA INDEX NAME)



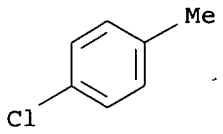
RN 17933-03-8 HCAPLUS
CN Boronic acid, (3-methylphenyl)- (9CI) (CA INDEX NAME)



RN 63139-21-9 HCAPLUS
CN Boronic acid, (4-ethylphenyl)- (9CI) (CA INDEX NAME)



IT **106-43-4 623-12-1**
RL: RCT (Reactant)
(reaction of, with diborane in presence of alk. metals)
RN 106-43-4 HCAPLUS
CN Benzene, 1-chloro-4-methyl- (9CI) (CA INDEX NAME)



RN 623-12-1 HCAPLUS
CN Benzene, 1-chloro-4-methoxy- (9CI) (CA INDEX NAME)